Version

6

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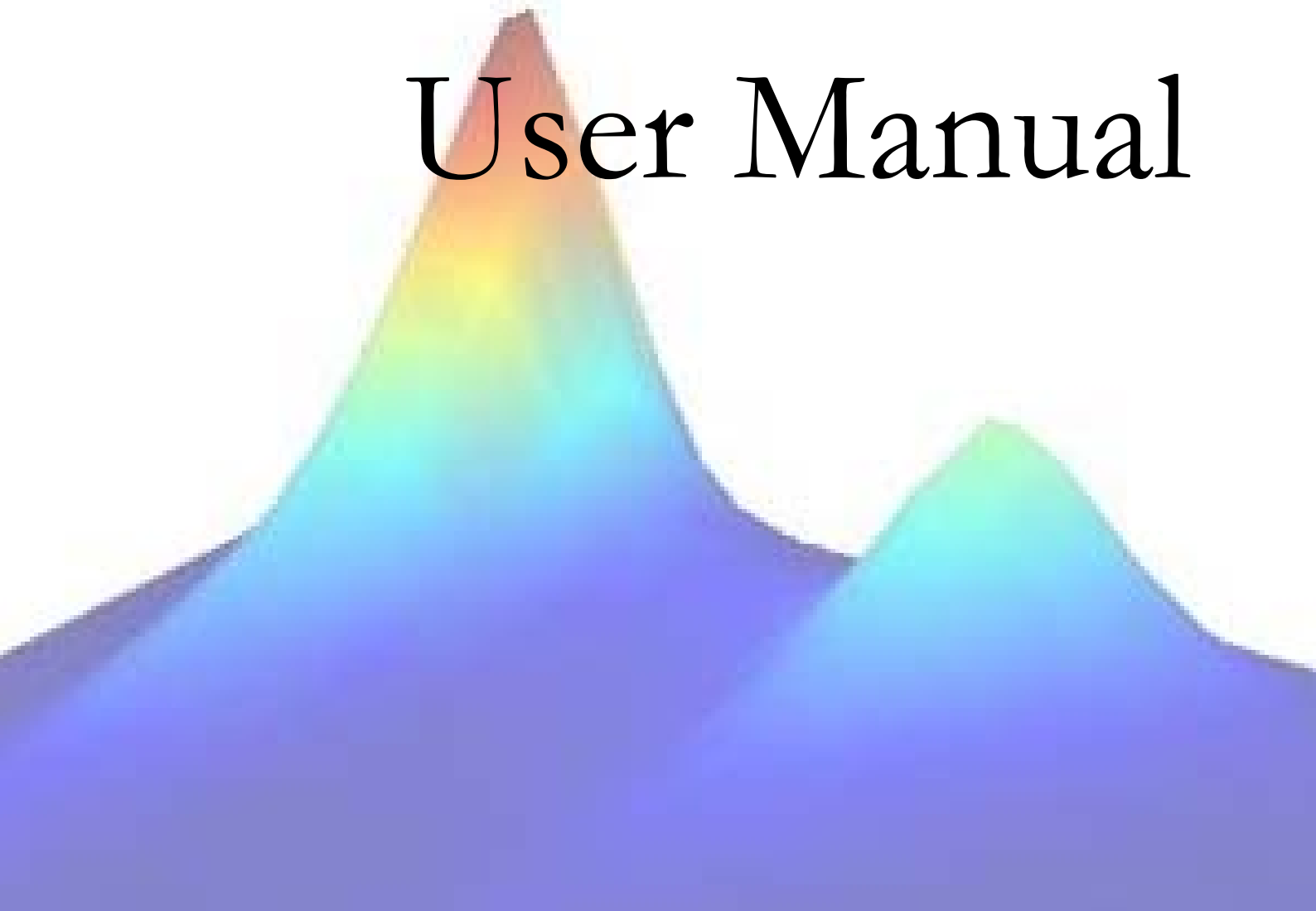
EBSD & MISORIENTATION CORRELATION FUNCTION

User Manual



This software was originally written to study the grain misorientation in relation with the nearest neighbor's mutual distance using electron back-scattered diffraction measurements. I invite you to read "Spatial correlation in grain misorientation distribution, B. Beausir, C. Fressengeas, N.P. Gurao, L.S. Tóth, S. Suwas, Acta Materialia 57 (2009) pp. 5382-5395".

Since this work, further developments have been performed; several "special" quantities can be extracted from the EBSD measurements such as: the length and orientation of the boundaries between next-neighbours, the number of interconnected first neighbours around a grain…as an example, see "Effect of grain shape on next-neighbour misorientation distribution due to grain refinement by severe plastic deformation, L.S. Tóth, B. Beausir, C. Gu, Y. Estrin, N. Scheerbaum, C.H.J. Davis, Acta Materialia 58 (2010) pp.6706-6716"

This software is frequently upgraded; the new versions will be available on my homepage: http://benoitbeausir.free.fr/ on the "downloads" page. Also if you use this program and obtain suspicious results, or if you need particular information not available in the current version, please address your comments at:

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Nilesh P. Gurao (Department of Materials Engineering, Indian Institute of Science, Bangalore, India), Robert Chulist (Institut für Strukturphysik, Technische Universität Dresden, Dresden, Germany) and Chengfan Gu (Department of Materials Engineering, Monash University, Clayton, Australia) have kindly provided the three examples given with this manual.

B.B. thanks the Alexander von Humboldt Foundation for his research fellowship.

Contents

1 - Get Started

Install

Execute EBSDmcf_v#_L#_setup.exe and follow the instructions.

Package content

The package contains the following files:

- EBSDmcf.exe ..... executable file of the main program
- EBSDmcf.m ..... matlab plotting file
- BFG09.pdf ..... you have to read it
- TBG10.pdf ..... you have to read it
- ECAP_Cu_TD_1pass.ctf ..... data file example 1
- Compressed_titanium.ang ..... data file example 2
- SMA_tetra.ctf ..... data file example 3

Input data file

Data are taken from EBSD measurements, typically from TSL or Channel 5 Software. Simply export your data in the usual formats of these software:

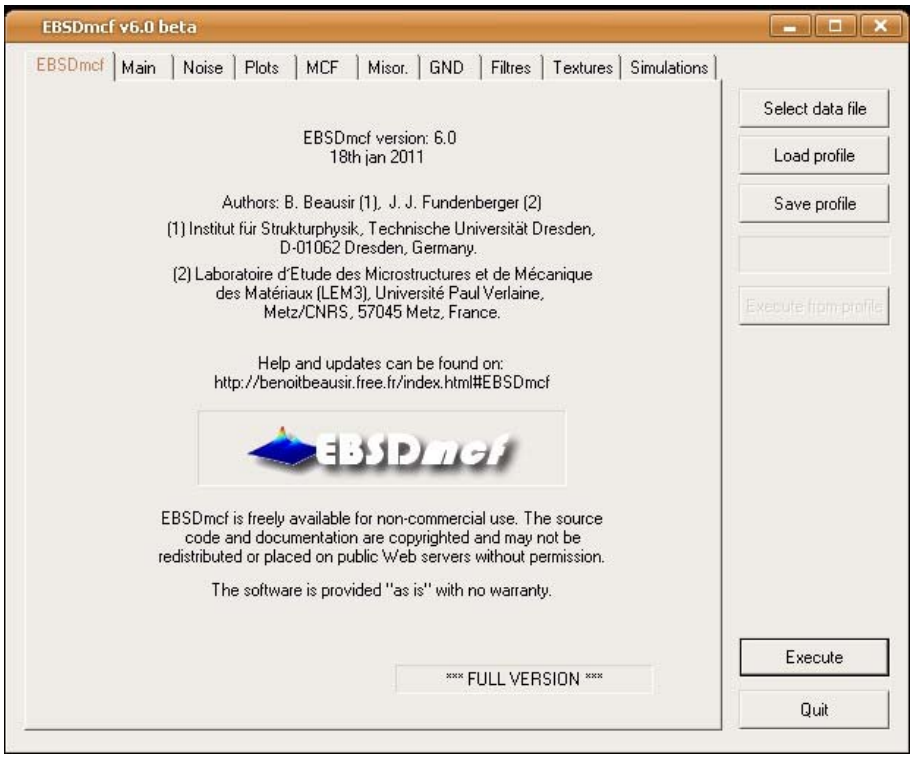
- From TSL, data have to be exported as *.ANG file format
- From Channel 5, data have to be exported as *.CTF file format

Three examples are given:

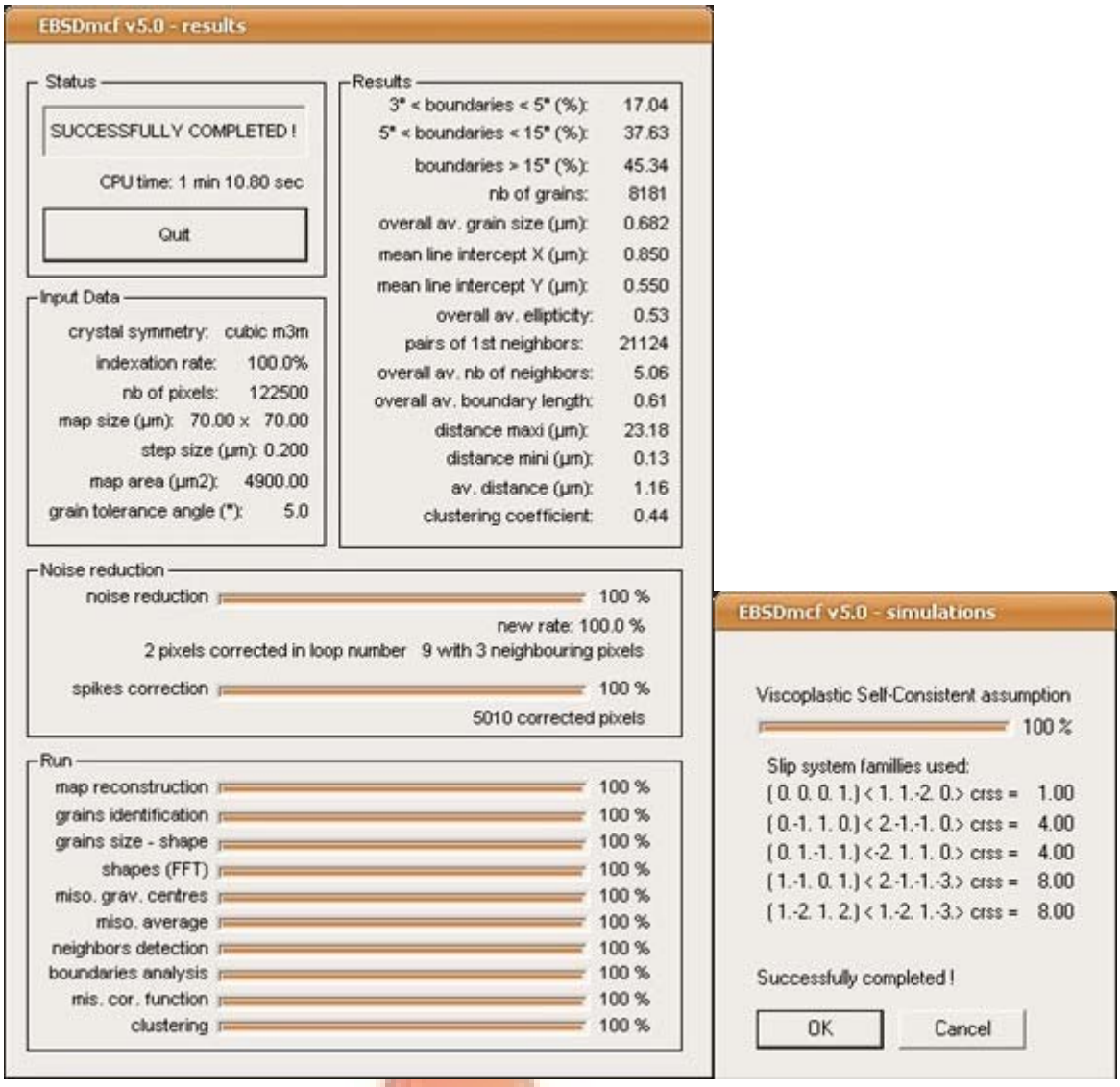
- ECAP_Cu_TD_1pass.ctf
- Compressed_titanium.ang
- SMA_tetra.ctf

Run the program

- Execute EBSDmcf.exe, the main dialog box appears:



- Choose your parameters in the differents tabs (see details after)
- Select your data file
- Click on execute, the “results” and the simulations (if required) boxes appears, please wait for the end of the run.
- Note, the parameters can be saved and loaded for subsequent runs ("Load profile" and "Save profile" buttons), to run a calculation from profile, frist select the data file, then load your profile (.pfl, ASCII) and clic on the "Execute from profile" button

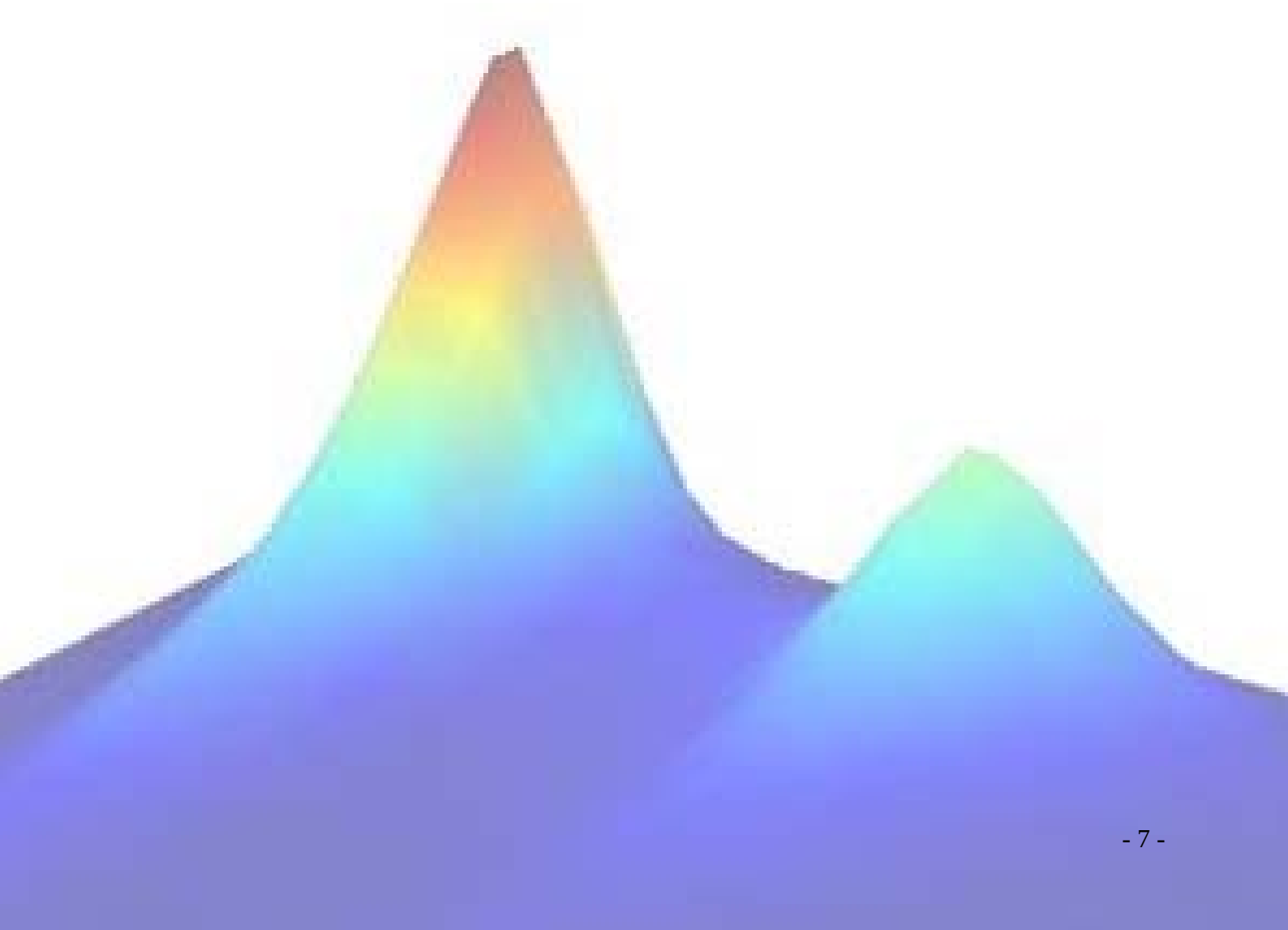


Restrictions

There are some restrictions according the version, restrictions on input parameters, features, output files and output maps. There are three levels of restriction, namely FULL VERSION(L0), RESTRICTED VERSION(L1) and SHAREWARE VERSION(L2)

Features	**L2**	**L1**	**L0**
Noise Reduction	✓	✓	✓
EBSD Parameters	✓	✓	✓
Filters			
Shapes	✓	✓	✓
Grain sizes	✓	✓	✓
Neighbors	✗	✓	✓

Cluster	✗	✗	✓
Links	✗	✗	✓
MCF Parameters	✓	✓	✓
Special Miso			
From particular orient.	✓	✓	✓
Gravity centre	✗	✗	✓
Average	✓	✓	✓
Dev. Ideal Orientations	✓	✓	✓
Simulations	✗	✓	✓



2 - Outputs

Maps

There are several plotted maps in BMP format

Files	L2	L1	L0	Map descriptions
01_MAP_BC.BMP	✓	✓	✓	Bands Contrast
02_MAP_MAD.BMP	✓	✓	✓	MAD
03_MAP_BS.BMP	✓	✓	✓	Bands Slopes
04_MAP_IPF.BMP	✓	✓	✓	Inverse Pole Figure
05_MAP_EULER.BMP	✓	✓	✓	All Euler
06_MAP_BOUND.BMP	✓	✓	✓	Boundaries
07_MAP_FITEL.BMP	✓	✓	✓	Elliptical fitting
08_MAP_FIT_BOUND.BMP	✗	✓	✓	Boundaries fitting
09_MAP_NET.BMP	✗	✗	✓	Network
10_MAP_NEIGH.BMP	✗	✗	✓	Number of neighbors
11_MAP_LINKS.BMP	✗	✗	✓	Number of links
12_MAP_CLUSTER.BMP	✗	✗	✓	Cluster parameters
13_MAP_GRAV.BMP	✗	✗	✓	Miso. from gravity centres
14_MAP_SPECMISO.BMP	✗	✓	✓	Miso. from a specified orientation
15_MAP_MEAN.BMP	✗	✓	✓	Miso. from average grain orientation
16_MAP_IDEAL.BMP	✓	✓	✓	Miso. from ideal orientations
17_MAP_NRJ.BMP	✗	✓	✓	Energy map from simulations
18_MAP_CLST_DIS.BMP	✗	✗	✓	Cluster parameters with distance
19_MAP_NUM.BMP	✓	✓	✓	Map displaying the grain IDs
20_MAP_GND12.BMP	✗	✗	✓	Alpha12 map
21_MAP_GND13.BMP	✗	✗	✓	Alpha13 map
22_MAP_GND21.BMP	✗	✗	✓	Alpha21 map
23_MAP_GND23.BMP	✗	✗	✓	Alpha23 map
24_MAP_GND33.BMP	✗	✗	✓	Alpha33 map
25_MAP_GND_NORME.BMP	✗	✗	✓	norme of the alpha tensor map
26_MAP_GND_TOTAL.BMP	✗	✗	✓	Total GND map
27_MAP_PLAN.BMP	✗	✗	✓	Trace of selected plane map

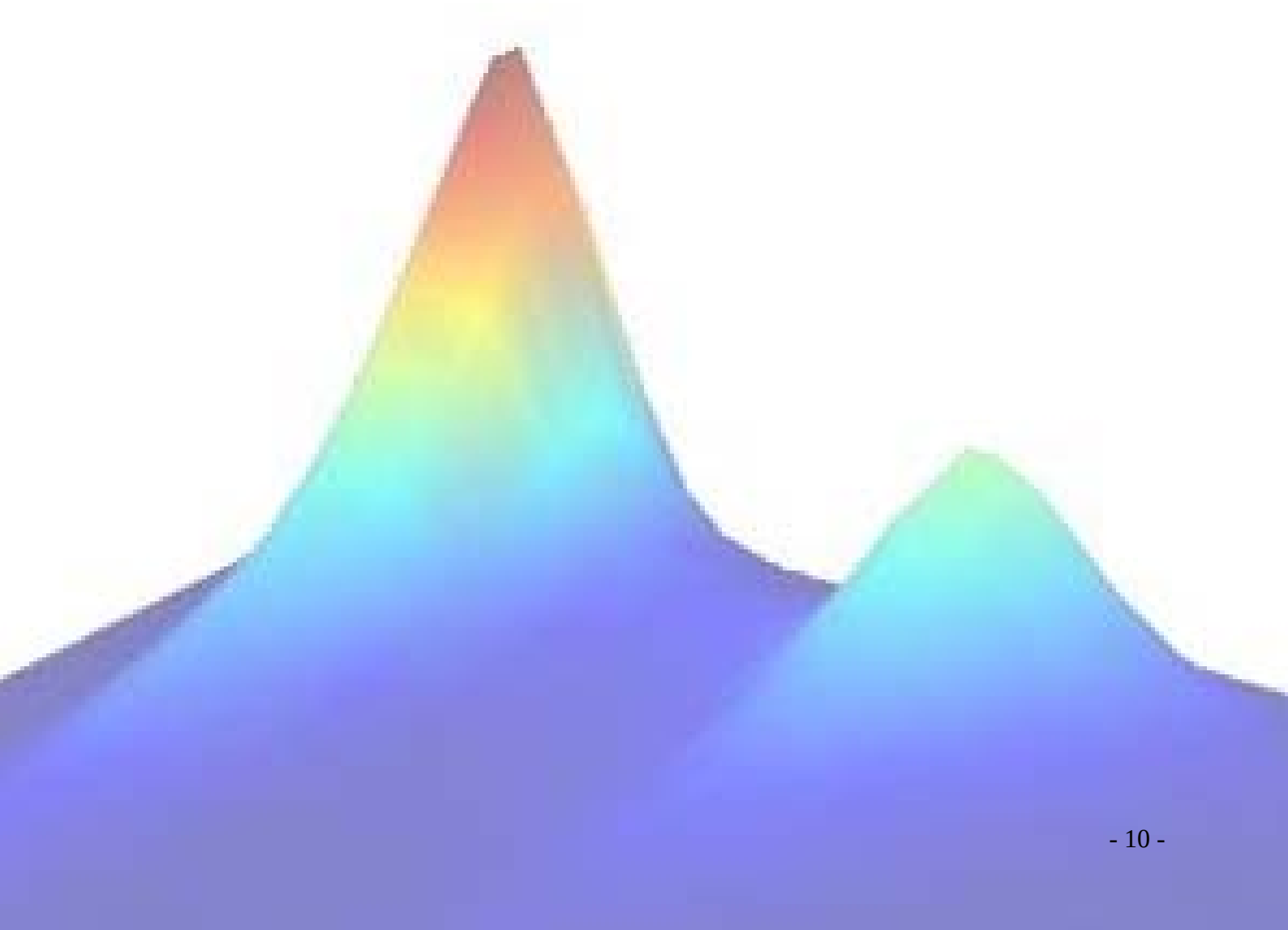
Files

There are several output files in ASCII or SVG formats

Files	L2	L1	L0	File descriptions
BOUND.OUT	✗	✓	✓	First-neighbours boundary characteristics
BOUND2.OUT	✗	✓	✓	First-neighbours boundary characteristics
CKPK.OUT	✗	✗	✓	For network analysis
DISTRIB_IDEAL.OUT	✓	✓	✓	Ideal orientation deviation distribution
DISTRIB_IDEAL_FILTRE.OUT	✓	✓	✓	DISTRIB_IDEAL.OUT only on selected grains
DISTRIB_IDEAL_REST.OUT	✓	✓	✓	DISTRIB_IDEAL.OUT on non-selected grains
FAST_FOURIER.OUT	✗	✗	✓	For grain shapes analysis
GRAINS.OUT	✓	✓	✓	Grain characteristics
GRAINS_FILTRE.OUT	✓	✓	✓	GRAINS.OUT only on selected grains
GRAINS_REST.OUT	✓	✓	✓	GRAINS.OUT on non-selected grains
GRAINSIZE.OUT	✓	✓	✓	Grain size distribution
GRAINSIZE_FILTRE.OUT	✓	✓	✓	GRAINSIZE.OUT only on selected grains
GRAINSIZE_REST.OUT	✓	✓	✓	GRAINSIZE.OUT on non-selected grains
MACKENZIE.OUT	✓	✓	✓	Misorientation distribution of the first neighbours
MCF.OUT	✓	✓	✓	Misorientation correlation function
MCFBL.OUT	✗	✗	✓	MCF but with boundary lengths
MIS_AXIS.OUT	✗	✓	✓	Misorientation axes between neighbors
MISOGRAV_SIZE.OUT	✗	✗	✓	Statistics on miso grav center with grain sizes
NEIGHBORS.OUT	✓	✓	✓	List of the first neighbours
NETWORK.OUT	✗	✗	✓	For network analysis
OLDGB.OUT	✓	✓	✓	For NNMD analysis see [TBG10]
PERTURB.OUT	✗	✗	✓	For grain shapes analysis
PIX2PIXmiso.OUT	✓	✓	✓	Pixel-to-pixel misorientation distribution
RESULTS.OUT	✓	✓	✓	Main input parameters and various statistics
ROUGHNESS.OUT	✗	✗	✓	For grain shapes analysis

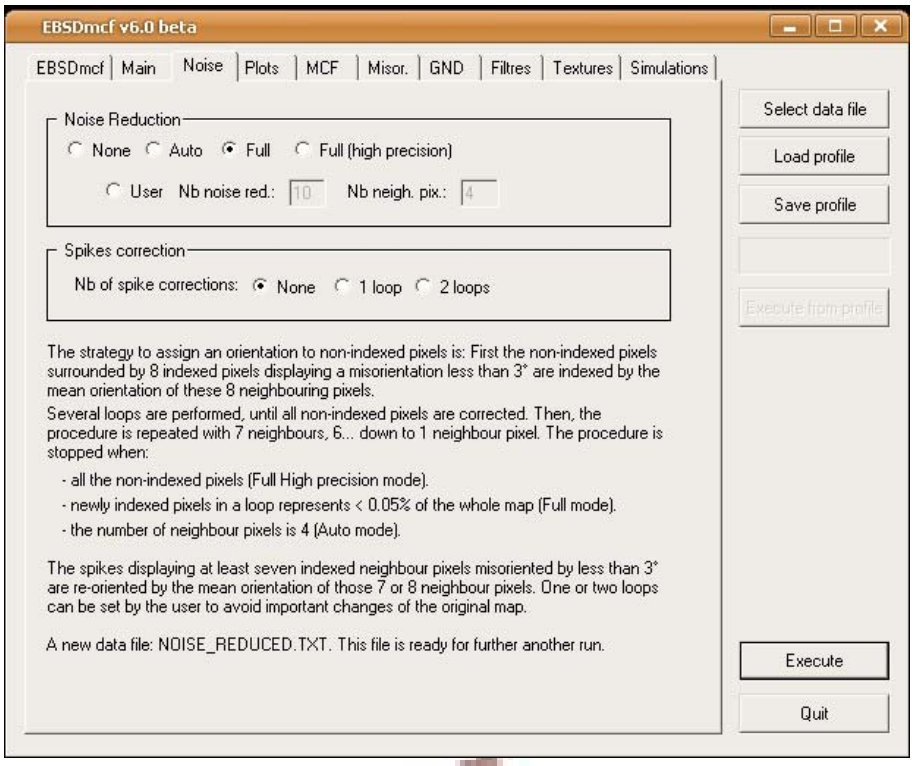
SIM_INPUT.OUT	✗	✓	✓	**Parameters used in the simulations**
SIMMAPS.OUT	✗	✓	✓	**Results of simulations**
temp.smt	✓	✓	✓	**Texture file of EBSD data**
SUBSET.TXT	✓	✓	✓	**Data file after subset file**
NOISE_REDUCED.TXT	✓	✓	✓	**Output noise reduction file**
PARAM.MTB	✓	✓	✓	**Parameters for Matlab plots**
FDP_*.SVG	✓	✓	✓	**Pole figures**
ODF_*_1.SVG*	✓	✓	✓	**ODF in phi1=const. sections**
ODF_*_2.SVG*	✓	✓	✓	**ODF in phi2=const. sections**
GRAINSIZE_AF.SVG*	✓	✓	✓	**Grain size distrib. area fraction**
GRAINSIZE_NB.SVG*	✓	✓	✓	**Grain size distrib. nb fraction**
PIX2PIXmiso.SVG*	✓	✓	✓	**Pix2pix miso. distrib.**
MACKENZIE.SVG*	✓	✓	✓	**Grain2grain miso. distrib.**
MCF.SVG*	✓	✓	✓	**M.C.F misor. sections**

* can be open with internet browsers or some imaging free software (like GIMP)



3 - Noise/spike reduction

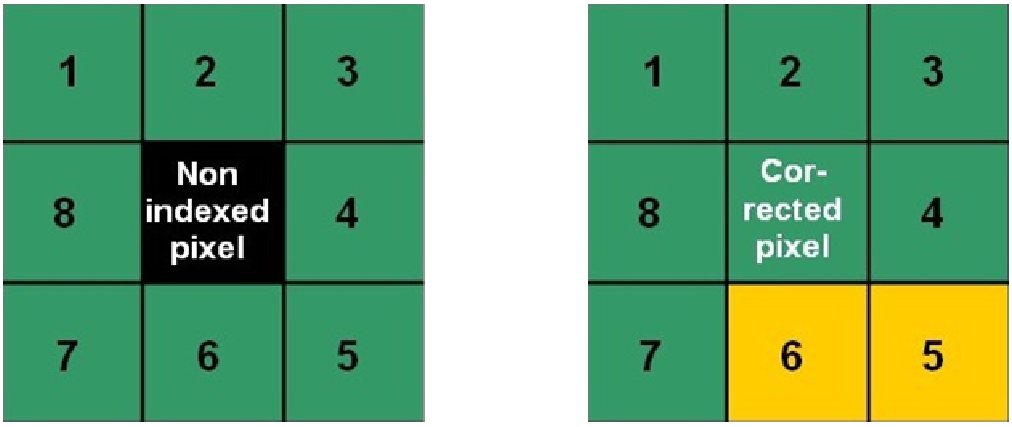
Noise reduction



There are four modes to perform the noise reduction: Full (high precision), Full, Auto or User. To avoid repeating the noise and spike corrections (see bellow), a new data file is created after the noise reduction and spikes correction: NOISE_REDUCED.TXT. This file can be read by the software for another run.

- FULL (High precision) mode

The strategy to assign an orientation to non-indexed pixels is: First the non-indexed pixels surrounded by 8 indexed pixels displaying a misorientation less than 3° are indexed by the mean orientation of these 8 neighbouring pixels. Several loops are performed, until all non-indexed pixels are corrected. Then, the procedure is repeated with 7 neighbours, 6… down to 1 neighbour pixel. The procedure is stopped when all the non-indexed pixels have been corrected. Example with 6 neighbour pixels:



- FULL mode

The strategy to assign an orientation to the non-indexed pixels is similar to the FULL mode except that when the number of newly indexed pixels in a loop represents less than 0.05% of the whole map the number of neighbouring pixels is decreased by 1. This mode can strongly reduces the time with respect to the full (high precision) mode.

- AUTO mode

The strategy to assign an orientation to the non-indexed pixels is similar to the FULL mode except that the number of neighbour pixels is limited to 4.

- USER mode

The user can set the number of correction loops and the number of neighbour pixels.

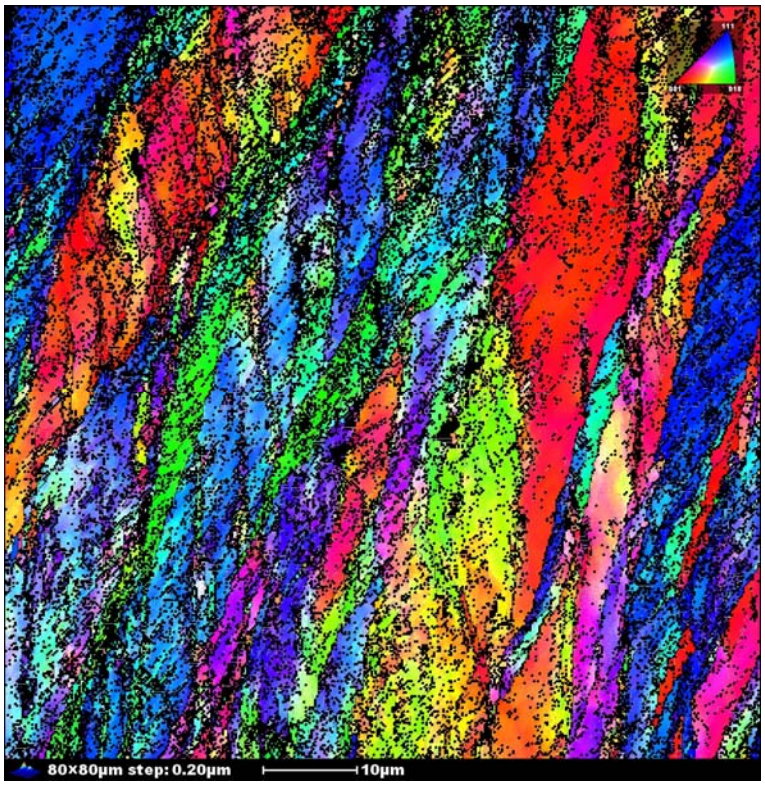
Spike correction

The strategy to assign a new orientation to a spike is as follows: The spikes displaying at least seven indexed neighbour pixels misoriented by less than 3° are re-oriented by the mean orientation of those 7 or 8 neighbour pixels. One or two loops can be set by the user. The procedure is limited to two loops to avoid important changes of the original map. See the figure bellow.

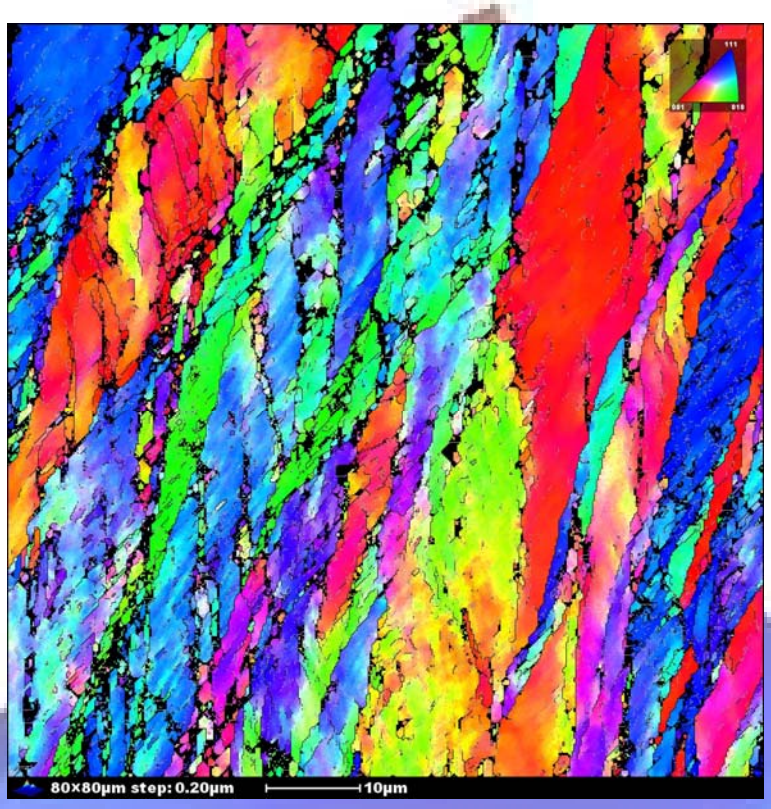
Initial: 2 spikes 1st spike correction loop 2nd spike correction loop

Example with ECAP_Cu_TD_1pass.ctf

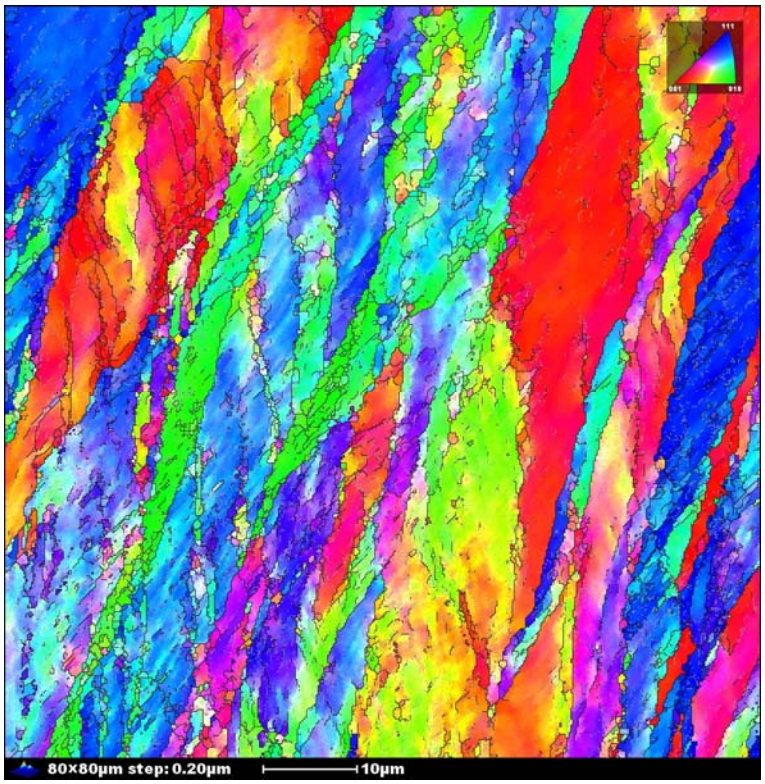
Initial 70% indexed



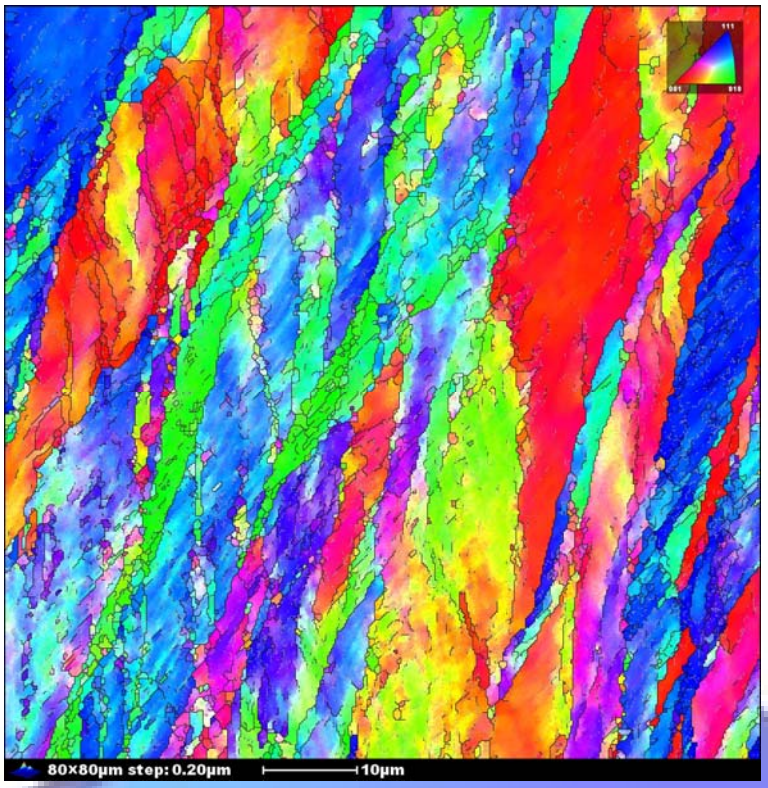
Corrected with AUTO mode: 91% indexed



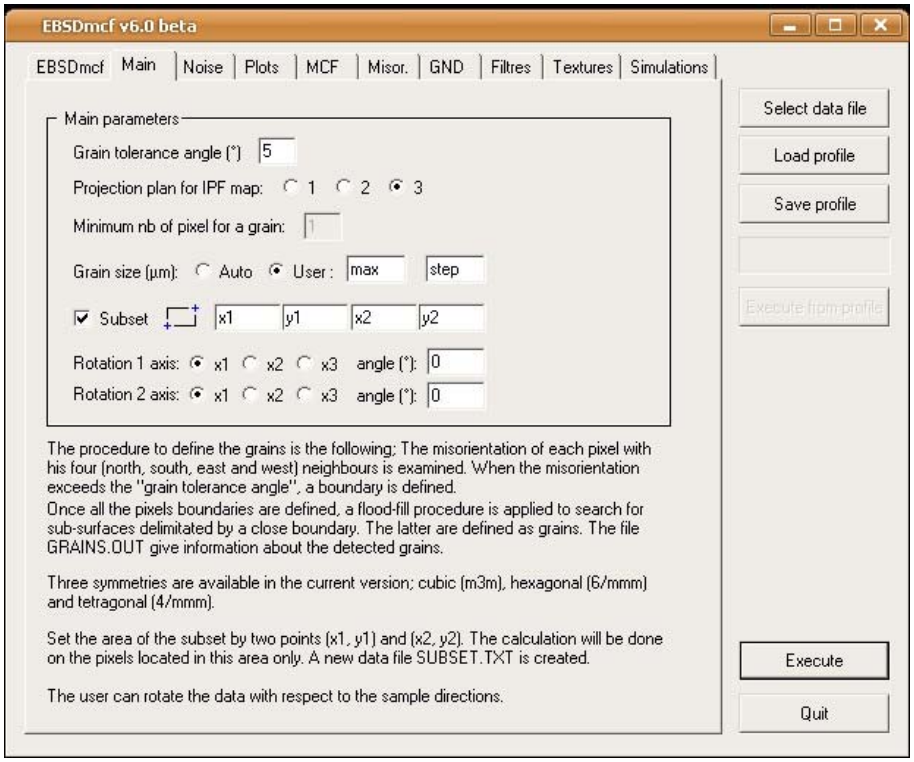
Corrected with FULL mode: 100% indexed



FULL (high precision) mode + Spikes correction



4 - Basic Options



Note: the options « minimum nb of pixel for a grain » is not available in this version

Grain Tolerance Angle and grain detection

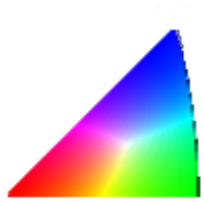
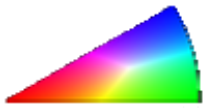
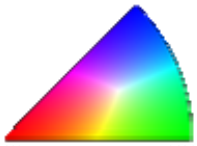
The procedure to define the grains is the following; The misorientation of each pixel with his four (north, south, east and west) neighbours is examined. When the misorientation exceeds the “grain tolerance angle”, a boundary is defined. Once all the pixels boundaries are defined, a flood-fill procedure is applied to search for sub-surfaces delimitated by a close boundary. The latter are defined as grains. The file GRAINS.OUT give information about the detected grains, there are seven columns in this file:

- 1. ID: the grain ID
- 2. Surface: surface of the grain
- 3. XG: x-coordinate of the grain gravity center
- 4. YG: y-coordinate of the grain gravity center
- 5. Phi1: Euler angle 1 (Bunge convention)
- 6. Phi: Euler angle 2 (Bunge convention)
- 7. Phi2: Euler angle 3 (Bunge convention)
- 8. grain size
- 9. ellipticity (see after for the definition)
- 10. angle of the fitted ellipse
- 11. average internal misorientation
- 12. clustering coefficient

- 13. clustering coefficient distance
- 14. number of links
- 15. number of neighbors
- 16. neighbor's ID

Inverse pole figure maps

The orientation of each pixel is projected in inverse pole figures with respect to one of the three sample directions. One colour is given to each pixel according the Maxwell's colour triangle [M61]. Three symmetries are available in the current version; cubic (m3m), hexagonal (6/mmm) and tetragonal (4/mmm): the IPF map is 04_MAP_IPF.BMP

Cubic (m3m) Hexagonal (6/mmm) tetragonal (4/mmm)

Another map with a color code corresponding to the euler angles is also plotted: 05_MAP_EULER.BMP

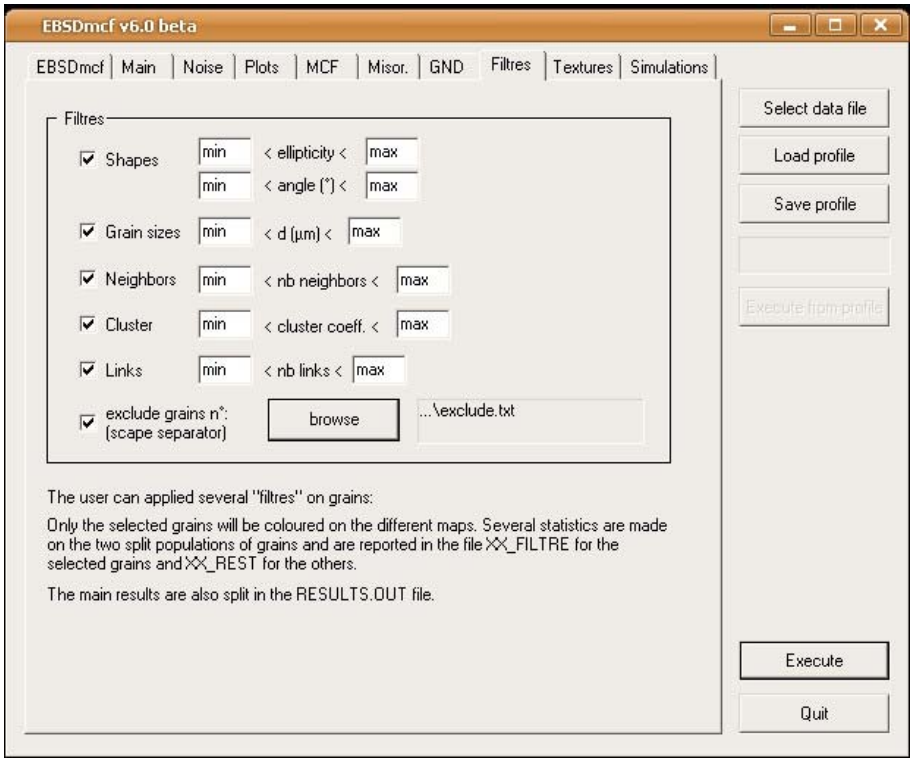
Subset mode

Set the area of the subset by two points (x1, y1) and (x2, y2). The calculation will be done on the pixels located in this area only. A new data file SUBSET.TXT is created.

Rotations

Please textures pages for explainations on rotations.

5 - Filtres



The user can applied several “filtres” on grains:

- On shapes: ellipticity and angle of the ellipses
- On grain sizes
- On the number of neighbors
- On the number of links
- On the cluster coefficients
- On the grain IDs (a ASCII file has to be prepared, it has to contain IDs of the grains (one per line).

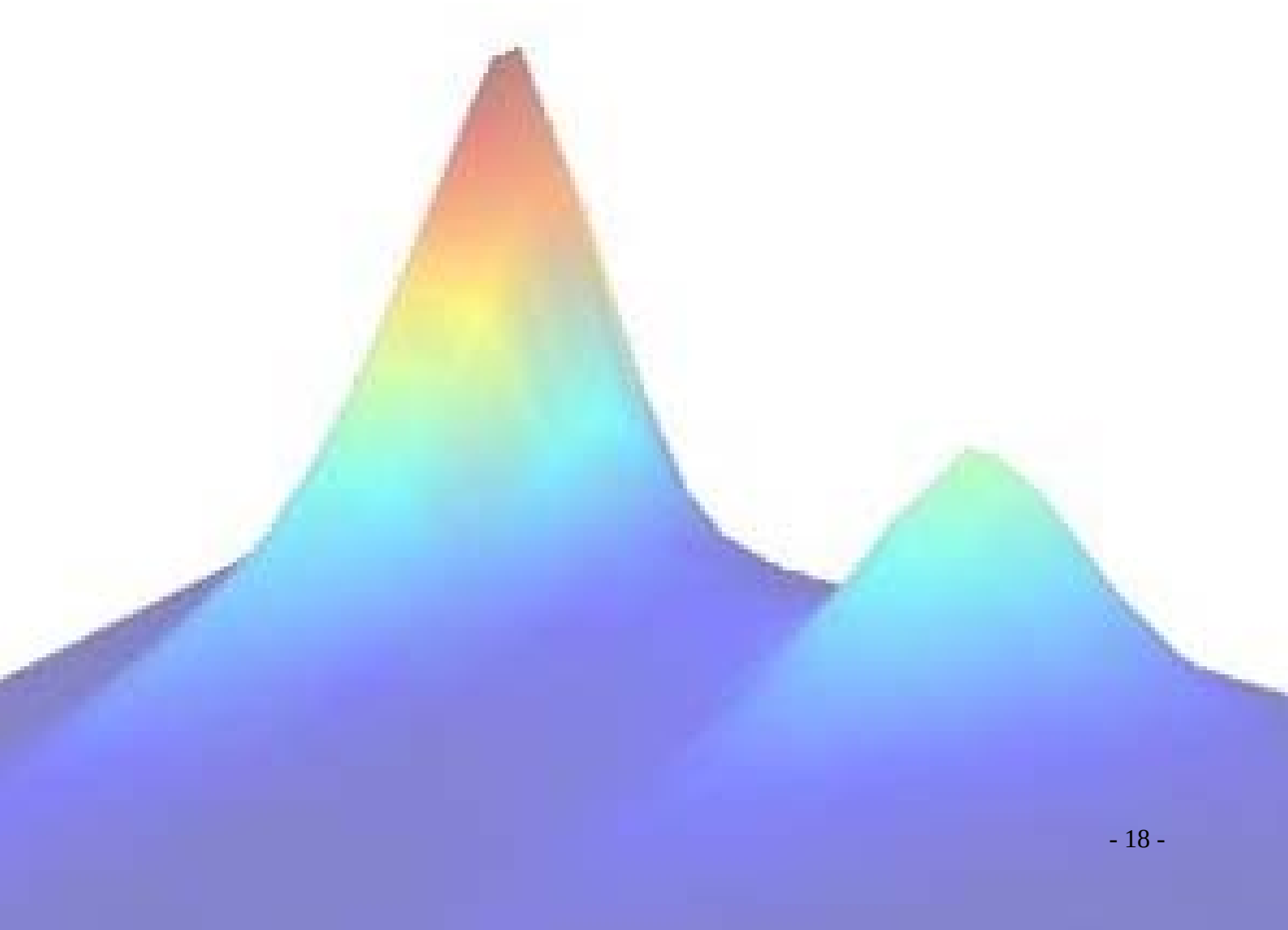
Only the selected grains will be coloured on the different maps. Several statistics are made on the two split populations of grains and are reported in the file XX_FILTRE for the selected grains and XX_REST for the others. Refer to the list of output file above.
The main results are also split in the RESULTS.OUT file

6 - First neighbours detection

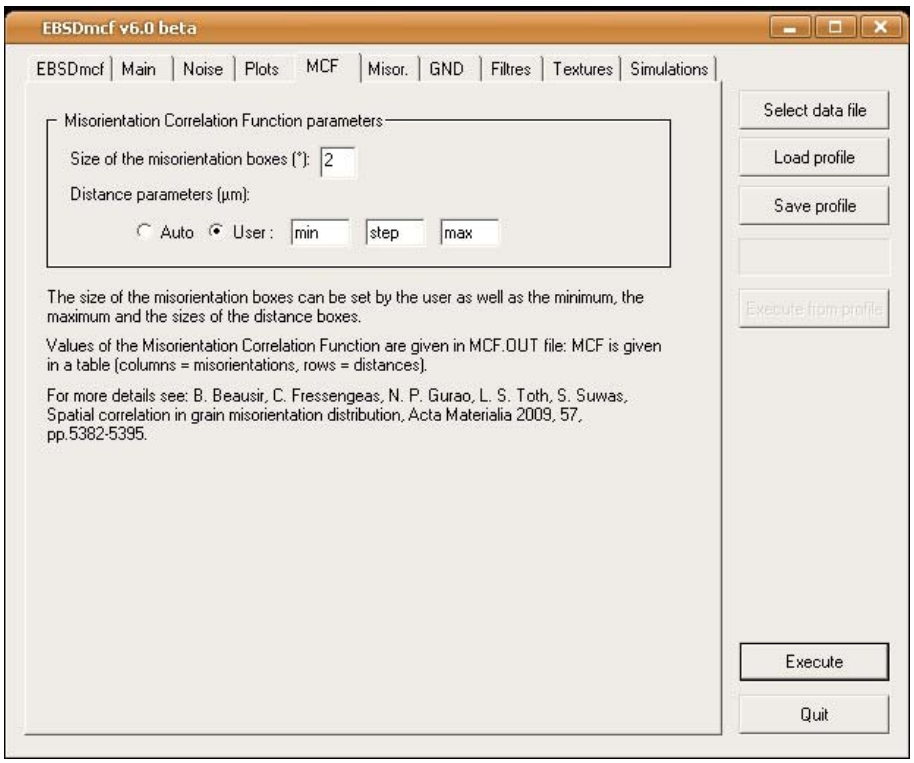
If a grain displays a boundary with another grain, these two grains are called “first neighbours”. They represent a “pair” of grains, or a pair of neighbours. The four neighbouring pixels are considered (North, East, West and South). The list of the first neighbours of each grain can be found in the NEIGHBORS.OUT file; by row: ID; number of neighbours (NbNbors); ID of the neighbours (ID_Neighbors).

The misorientation axes characteristics are contained in the MIS_AXIS.OUT file: six columns

- 1. x1, x-coordinate of the axis on inverse pole figure
- 2. x2, y-coordinate of the axis on inverse pole figure
- 3. theta (the corresponding misorientation value)
- 4. Miller index 1
- 5. Miller index 2
- 6. Miller index 3



7 - Misorientation Correlation Function (MCF)

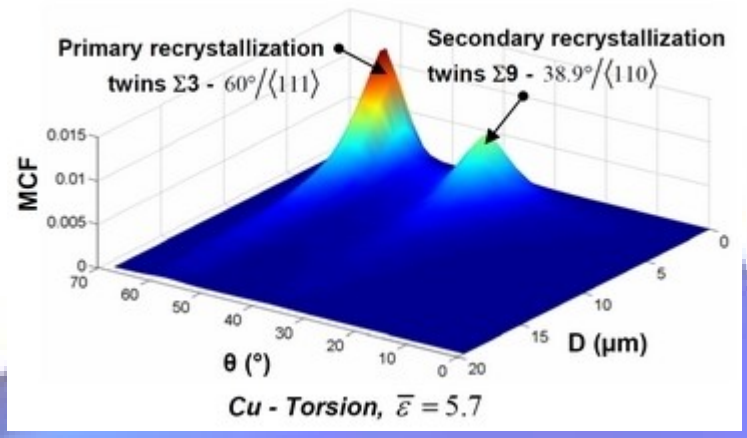


Please refere to Beausir et al. [BFG09]

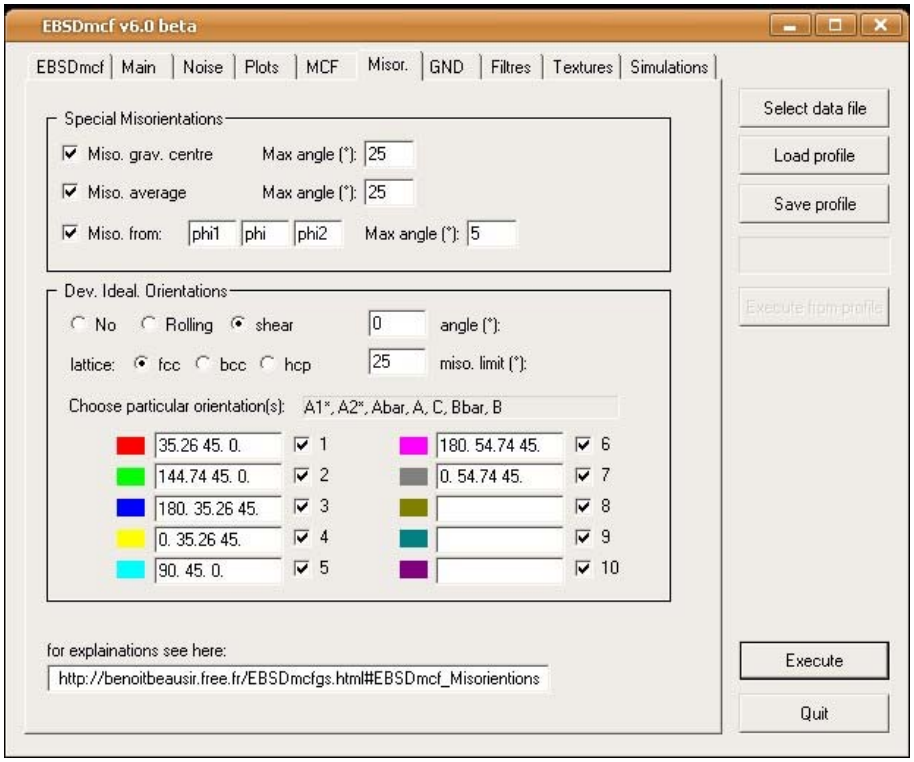
The size of the misorientation boxes can be set by the user as well as the minimum, the maximum and the sizes of the distance boxes.

Values of the Misorientation Correlation Function are given in MCF.OUT file: MCF is given in a table (columns = misorientations, rows = distances).

For more details see Beausir et al. [BFG09]



8 - Misorientations



Misorientations distributions

Two ways are proposed to present the misorientation distribution, namely pixel-to-pixel and grain-to-grain.

The pixel-to-pixel is calculated from the misorientation between pixels and their four neighbouring pixels (North, South, East and West) and the results are given in the PIX2PIXmiso.OUT file.

The grain-to-grain misorientation distribution is calculated from the average orientation of grains. Then the misorientation between orientations of grains and their neighbors is calculated. The results are given in the MACKENZIE.OUT file.

Misorientations from the average grain orientation

A map 14_MAP_SPECMISO.BMP displaying the misorientation with respect to the average orientation of each grain is created, the corresponding color code is the following:

0° max angle

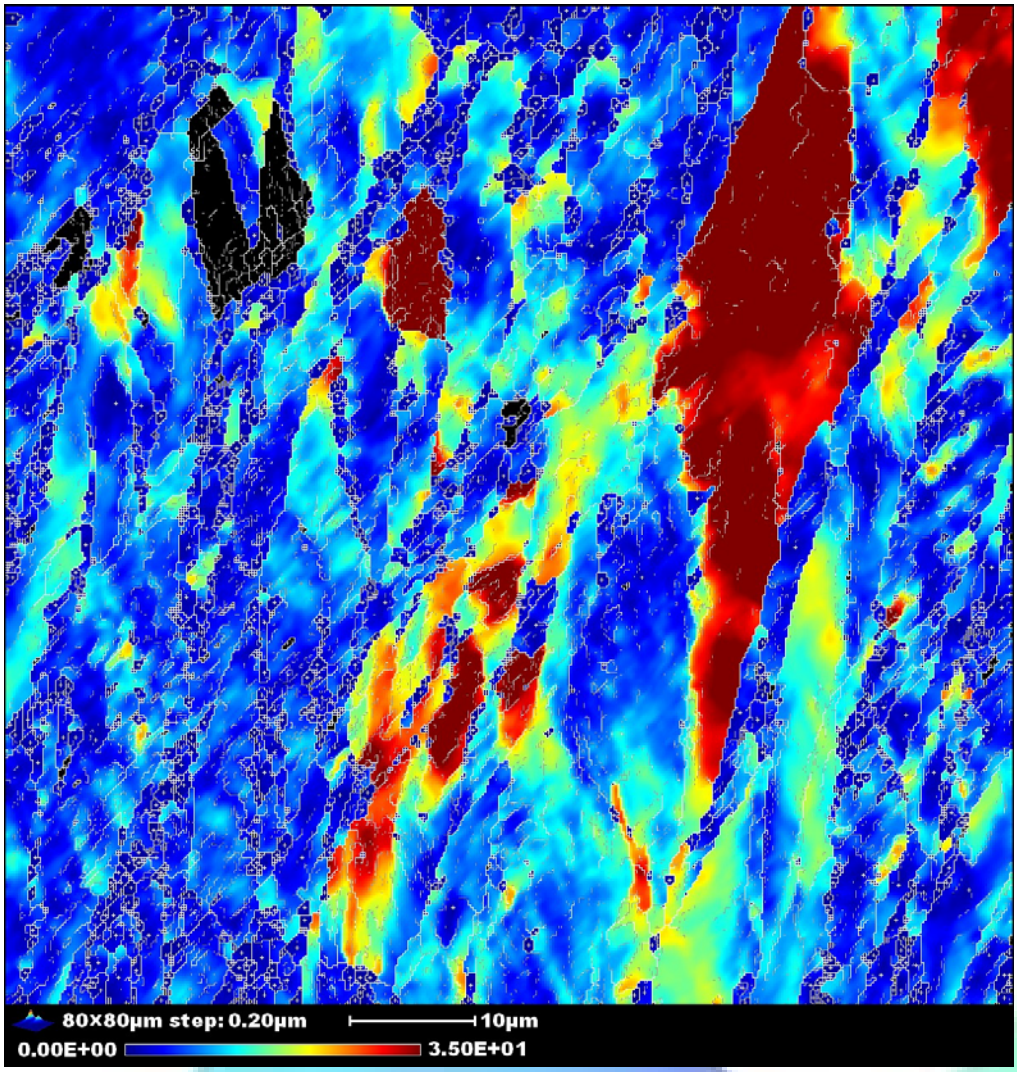
Misorientations from a single orientation

A map 15_MAP_MEAN.BMP displaying the misorientation with respect to a user specified orientation is created, the corresponding color code is the following:

0° max angle

Misorientations from the grain gravity centre

A map 13_MAP_GRAV.BMP displaying the misorientation with respect to the orientation of gravity centre of each grain is created.
Example with ECAP_Cu_TD_1pass.ctf:



Note that when the gravity centre of a grain is outside of the grain, the grain is coloured in black, when the misorientation exceed the maximum angle specified by the user the color correspond always to the maximum, i.e “red-brown”. The gravity centres are indicated by small white crosses.

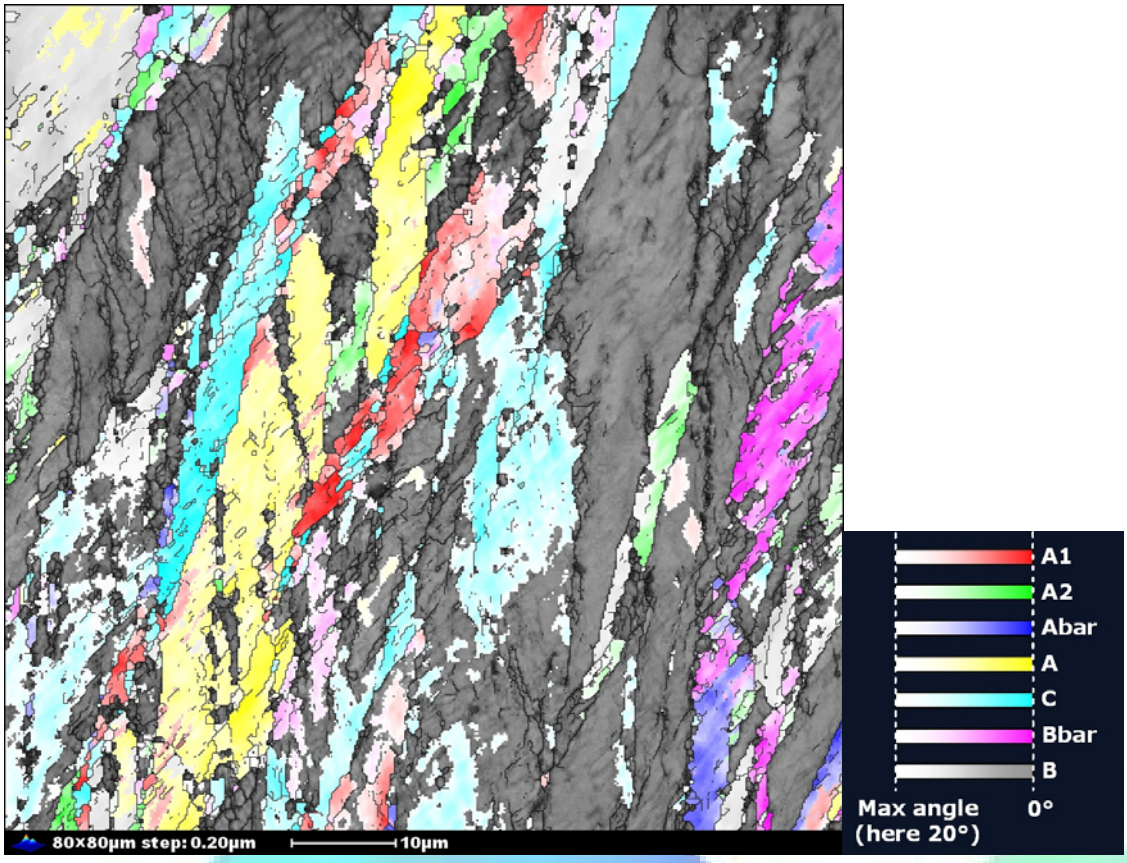
Misorientation with “Ideal orientations”

Misorientation of each pixel with ideal orientations is calculated, the nearest ideal orientation is selected, the user can set the limit of misorientation for which the pixel is considered near to an ideal orientation. The distribution of misorientation is write in DISTRIB_IDEAL.OUT for each selected ideal orientations, the distribution is given with respect of the total number of pixel in the map.

A map is also plotted, 16_MAP_IDEAL.BMP where the pixels close to an ideal orientations are coloured as in the Tables below, when a pixel is not near to an Ideal orientation, i.e. when the misorientation exceed the misorientation limit, the pixel is coloured according the band contrast.

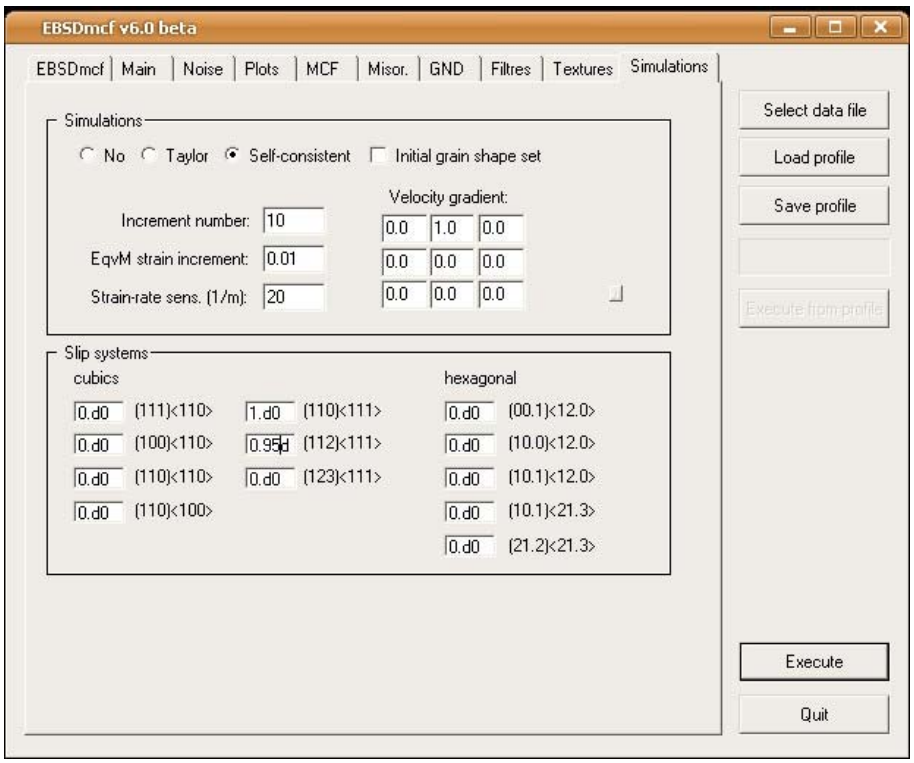
Note: be sure that your data are in the reference system of the ideal orientation defined in the table bellow, if not you can rotate your data (see before).

Example with ECAP_Cu_TD_1pass.ctf, color code corresponding to the ideal shear orientations in FCC metals (see also Table hereafter)



Shear + fcc: See Tóth et al. [TGJ88], shear direction is X, normal to shear plane is Y
Shear + bcc: See Baczynski and Jonas [BJ96], shear direction is X, normal to shear plane is Y
Shear + hcp: See Beausir et al. [BTN07], shear direction is X, normal to shear plane is Y
Rolling + fcc: See Hirsch and Lücke [HL88], rolling direction is X, normal direction is Z
Rolling + bcc: See Hölscher et al. [HRL91], rolling direction is X, normal direction is Z
Rolling + hcp: See Beausir et al. [BBK09], rolling direction is X, normal direction is Y

9 - Simulations, energy map...



Self-consistent [MCA87, MT94] and Taylor assumptions are available. For the self-consistent assumption the initial grain shape (ellipse fitting, see before) can be taken used as input of the simulations (the grain are circular by default). The plastic energy map 17_MAP_NRJ.BMP is plotted

When the reference stress of one family is different from zero the family will be considered in the simulation (if zero the family will be ignored).
The new orientations and the energy values of each grains are written in SIMMAPS.OUT.

The color bar corresponding to the plastic energy map is the following:

min energy max energy

10 - Grain sizes and grain shapes

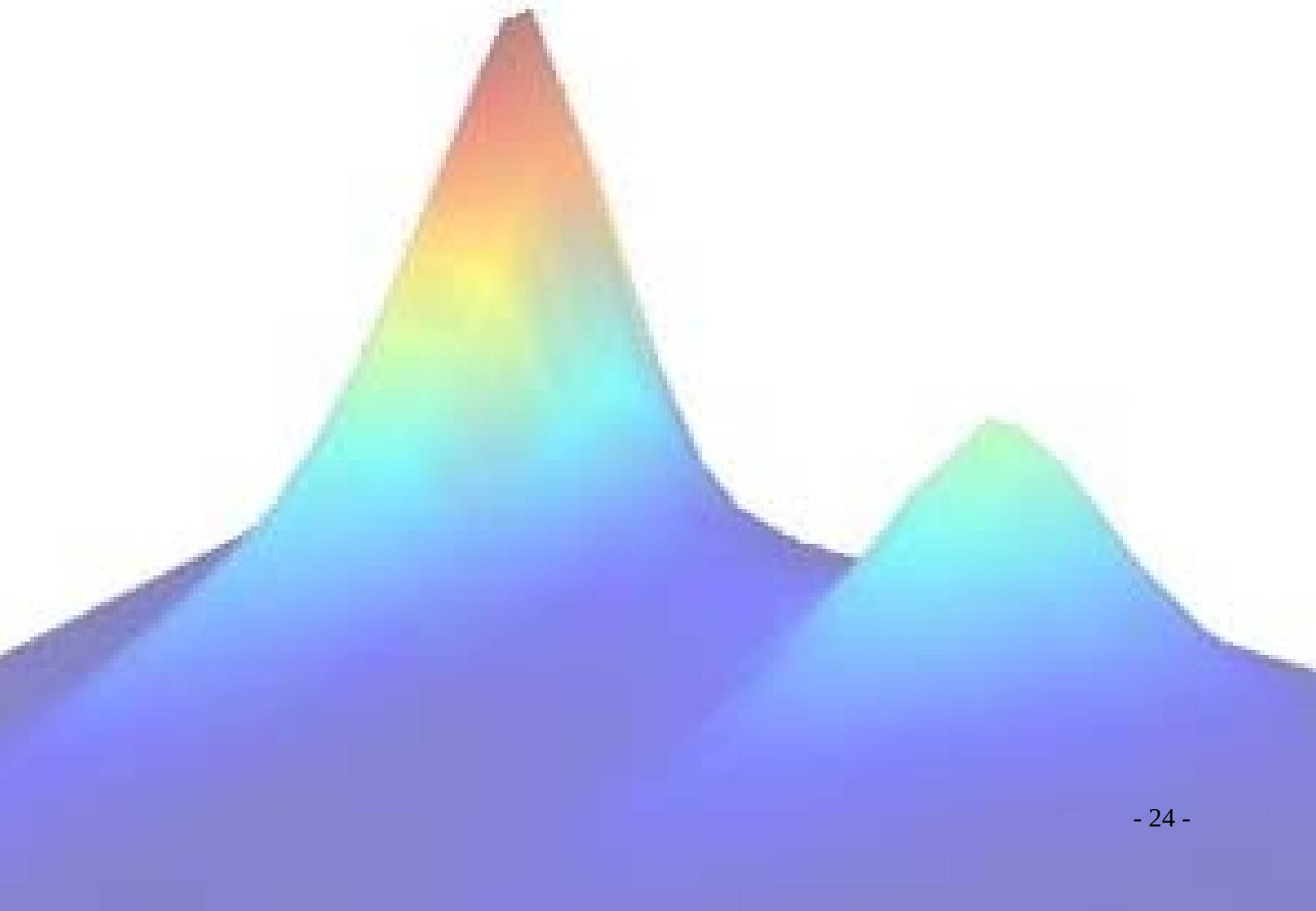
The grain size d is defined as follow: d = 2 * sqrt (S / pi)

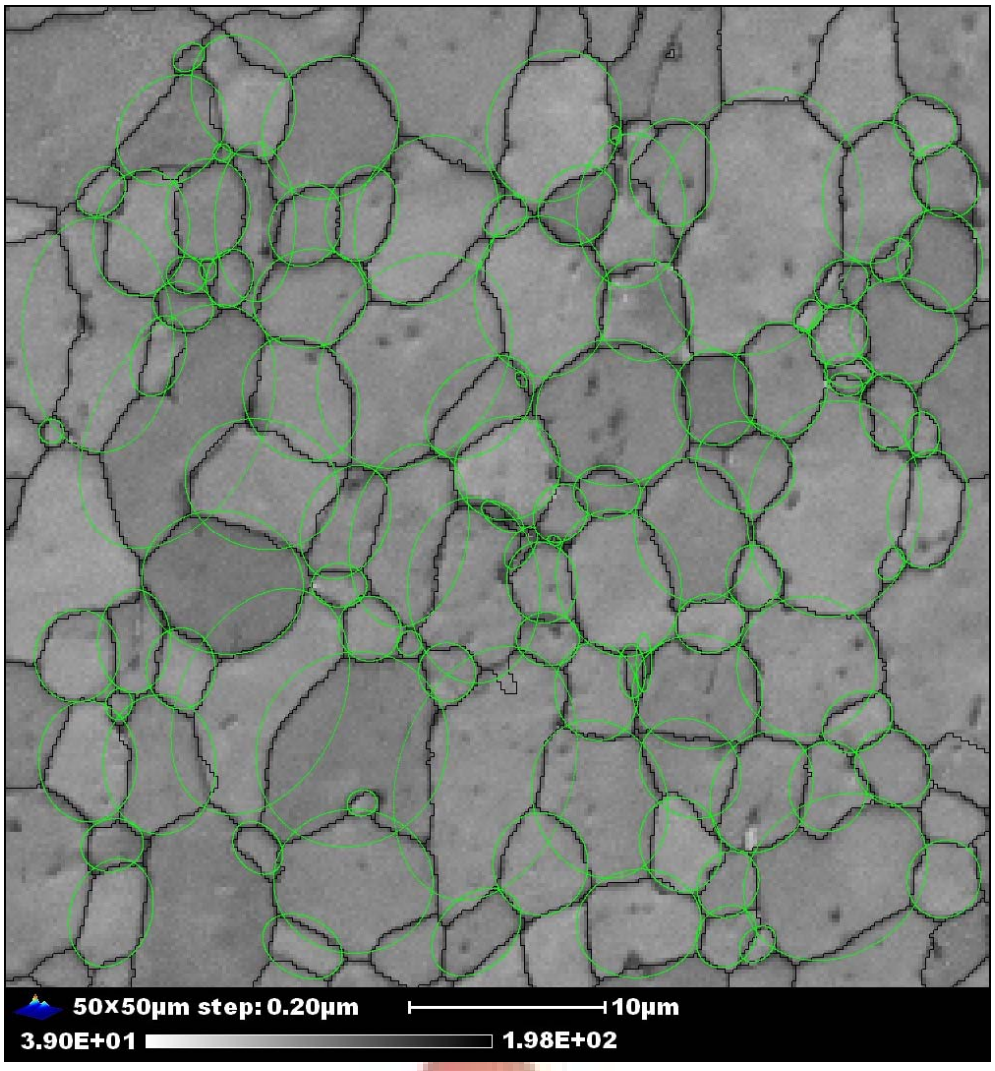
Where S is the surface of the grains. The results are given in GRAINSIZE.OUT. The size and the maximum of the histogram boxes can be set by the user. The Auto mode chooses the maximum grain size as maximum and 2 pixels as box sizes. The two column in GRAINSIZE.OUT give the number fraction and area fraction, respectively. The grain size is also calculated from line intercept method with respect to the X and Y directions. Each row (X) and Column (Y) of pixels is examined, the average distance between boundaries (according the Grain Tolerance Angle of the user) with respect to X and Y directions is calculated and given in the RESULS.OUT file and in the main window.

Ellipse fitting

Once the grains are detected and their gravity centres known, the grains are fitted by ellipses. From the fit the big axis a and the small axis b as well as the angle of the big axis with the direction 1 of the sample are obtained. Thus the ellipticity of each grains is calculated as follow: E = 1 - b / a

For a circle the ellipticity is zero and when a >> b the ellipticity tends to 1.
Note that the grains on the map borders are not considered





Fast Fourier Transformation

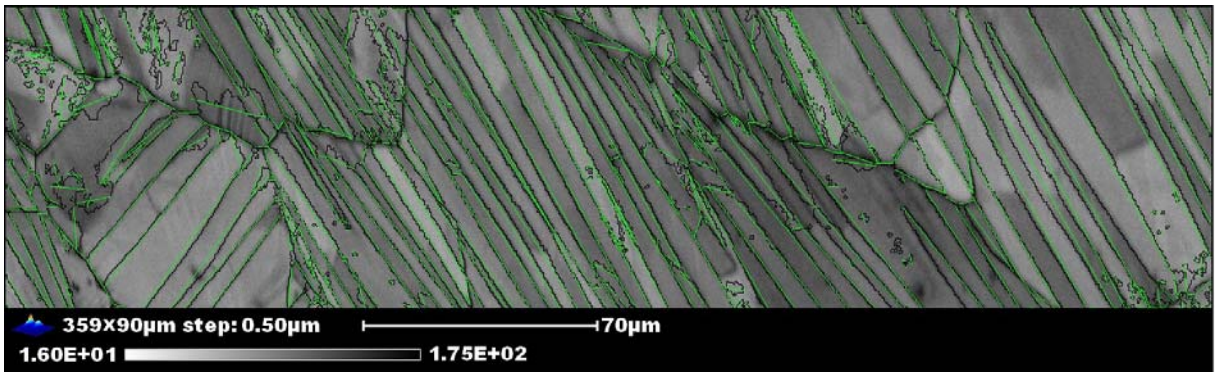
Not explained in the current version.

11 - Boundary analyses

The grain boundaries are approximated by straight lines at angle with axis 1 of the sample. This angle is reported in BOUND.OUT, Boundary characteristics are written in this file for pairs of first neighbours, in four columns:

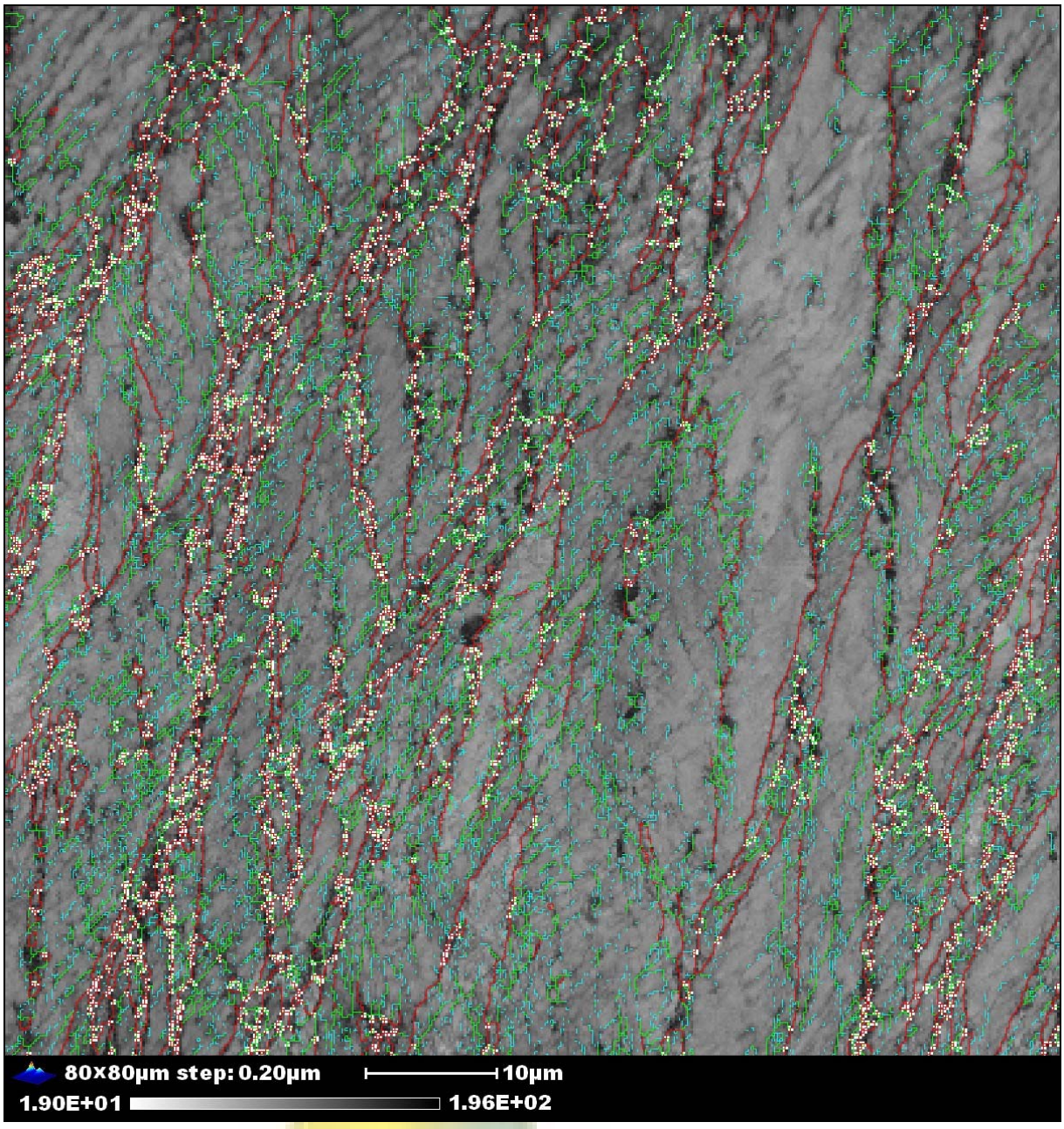
- 1. ID grain 1
- 2. ID grain 2 (the considered neighbour)
- 3. the length of their common boundary
- 4. the angle of this boundary with respect to the direction 1 of the sample

Example with SMA_tetra.ctf:



Note that the length of the boundaries are also indicated in BOUND.OUT. These lengths are not extracted from the approximated lines, but from the number of pixels constituting the boundaries.

The boundaries are also plot as with different colors as function of the misorientation angle, example with ECAP_Cu_TD_1pass.ctf

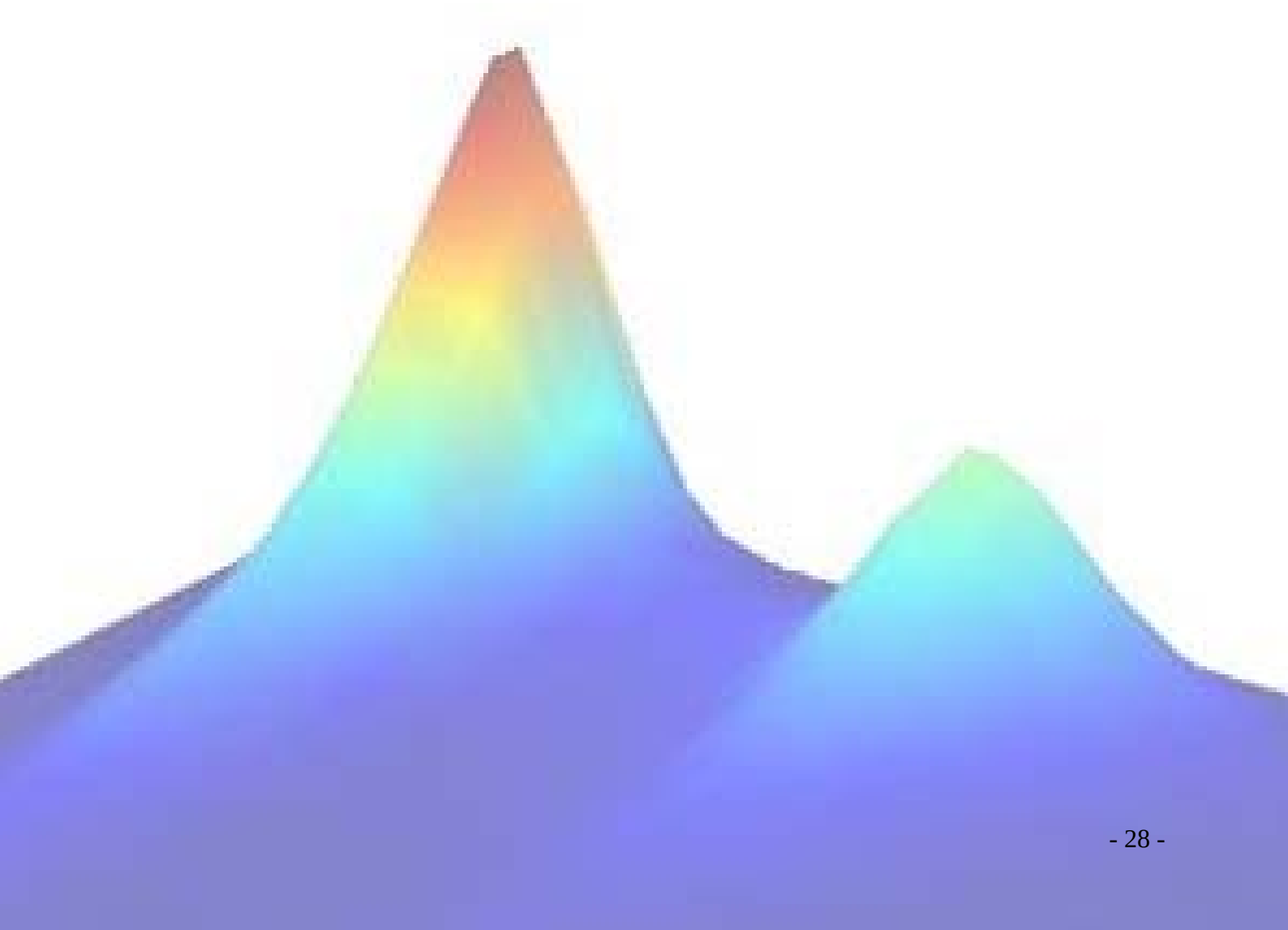


In red >15°, in green between 5 and 15° and blue between 3 and 5°. The white dots are the triple points.

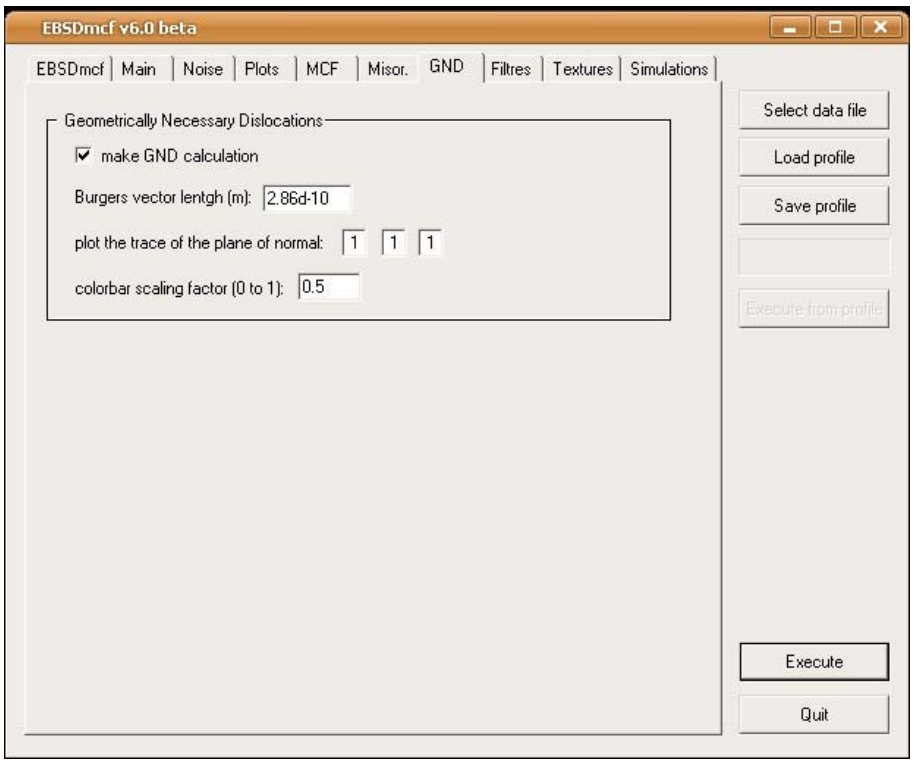
12 - Special features

Clustering coefficient

The clustering coefficient is not explained in the current version.

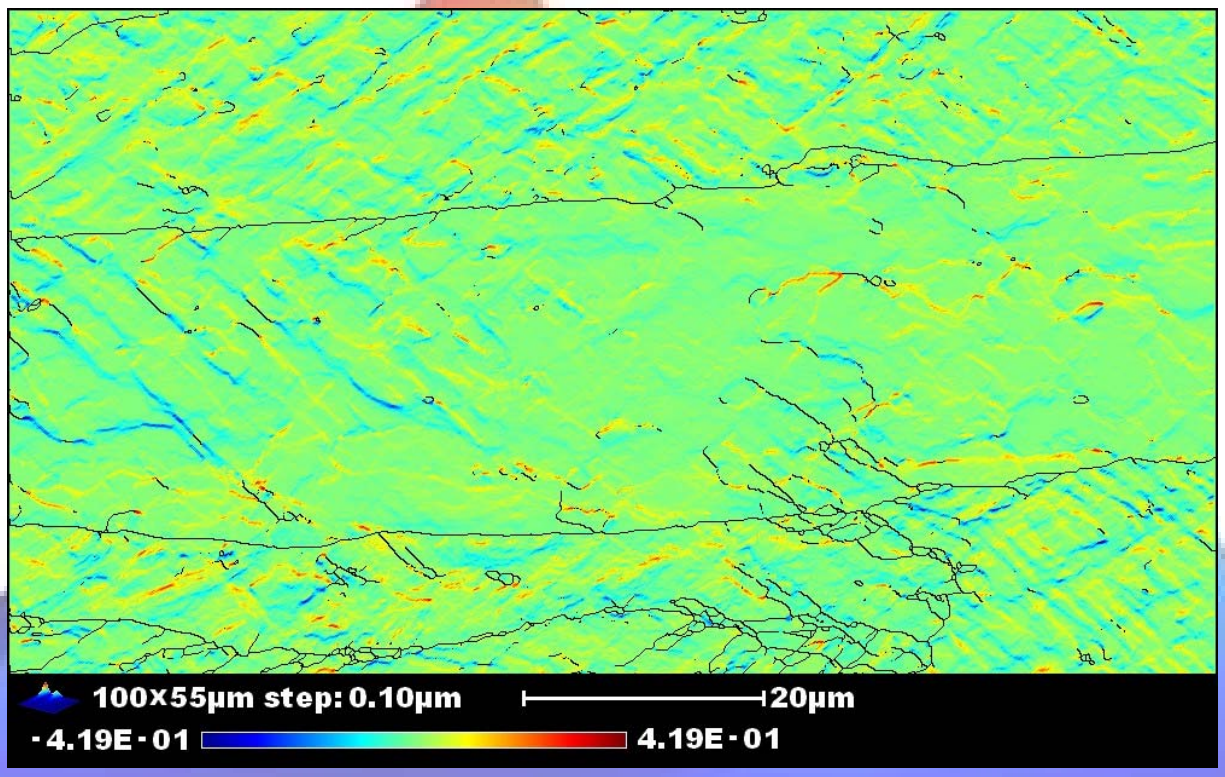


13 - Geometrically Necessary Dislocation

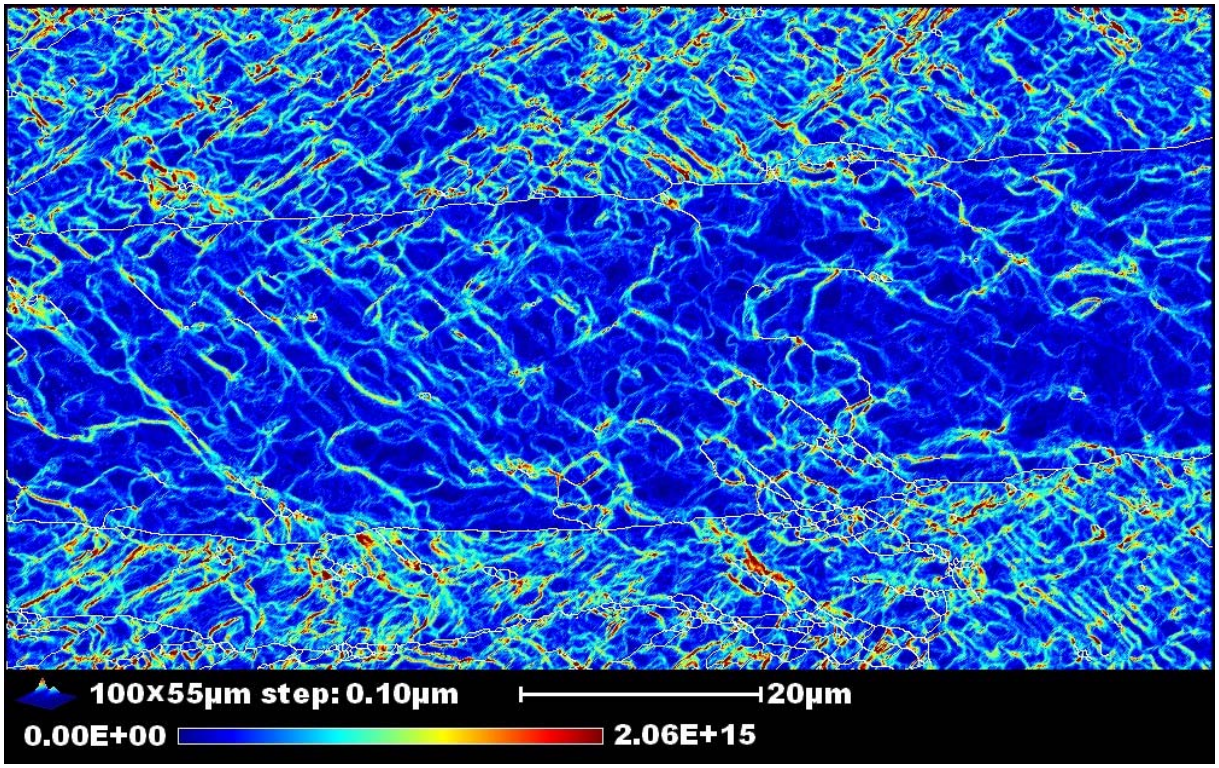


Geometrically Necessary Dislocation

Just an example for the moment, 21-component of the Nye tensor (µm-1)



Total gnd (m-2)



14 - Textures

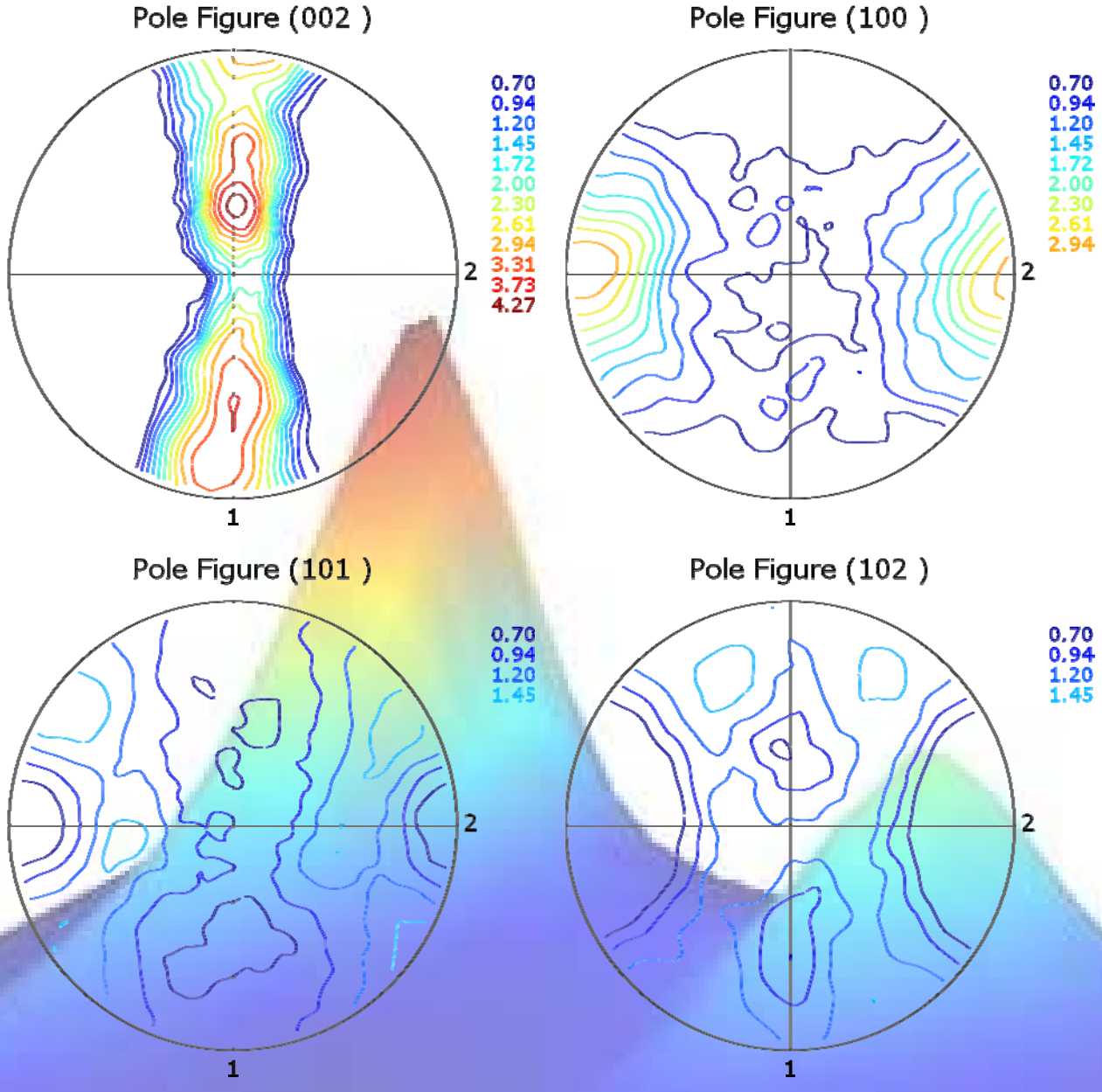
Texture rotation

The user can rotate the data with respect to the sample directions.

Pole figures

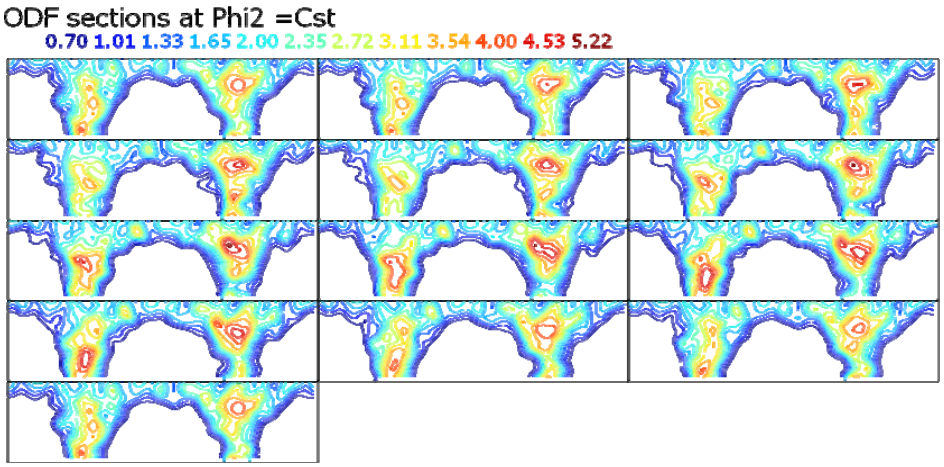
see the files .SVG and example bellow, more explainations are coming soon

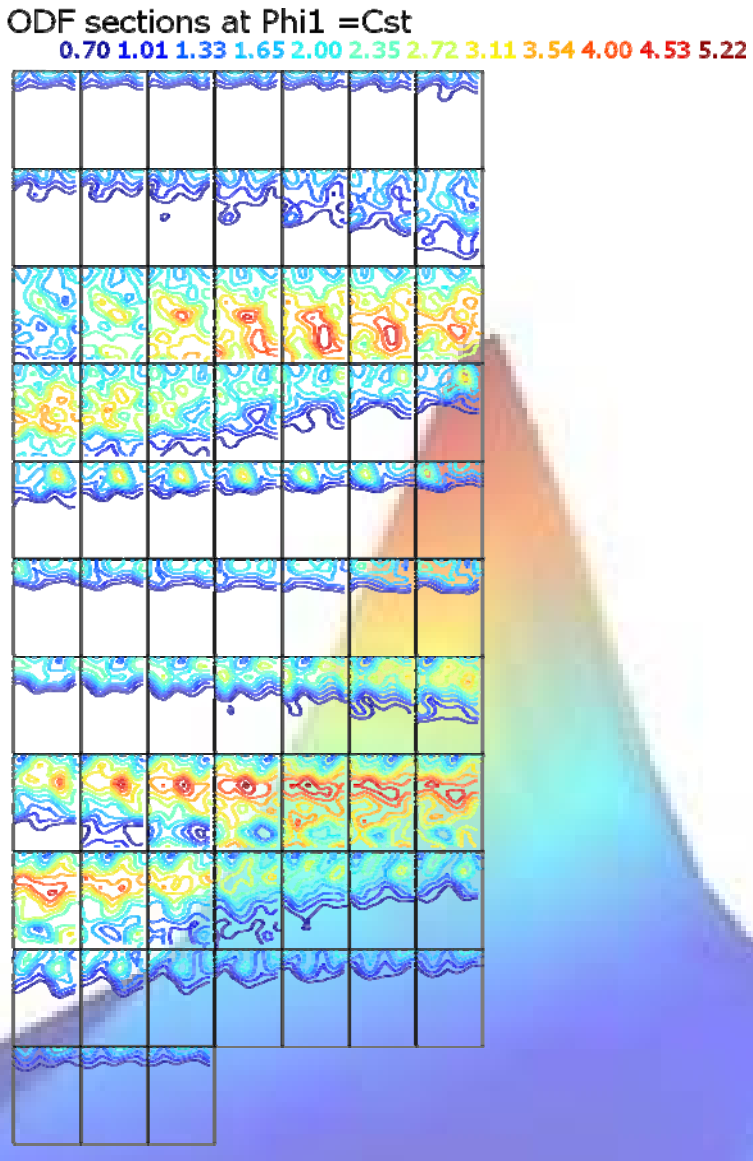
SVG files can be open with any internet browsers, the following plots has been checked in Google Chrome, another usefull freeware for SVG files is SVG-Edit (if you download it, simply open the html file with Firefox)



ODF sections

see the files .SVG and example bellow, more explainations are coming soon





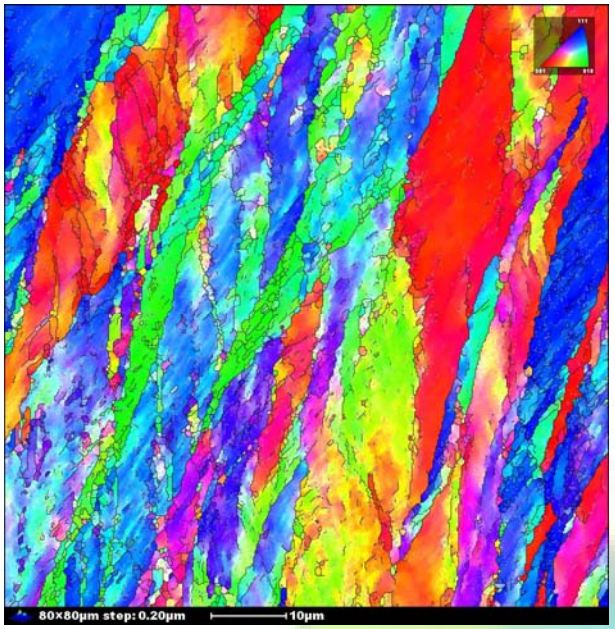
15 - Bugs

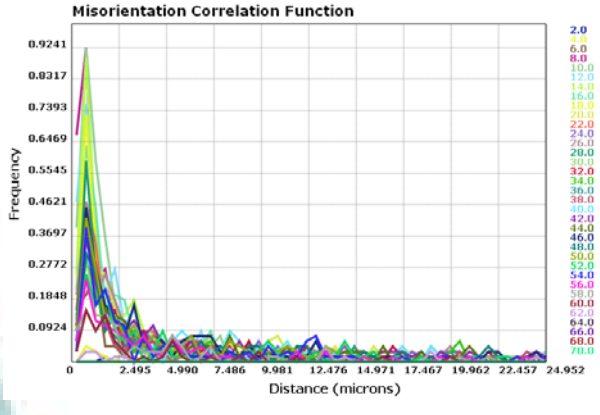
The results windows can be frozen (especially on windows) and thus the user can not see the progression of the computation. Just wait the end of the run. To close the programm before the end of a run you can simply go in the Task manager and stop the EBSD_MCF.exe processus.

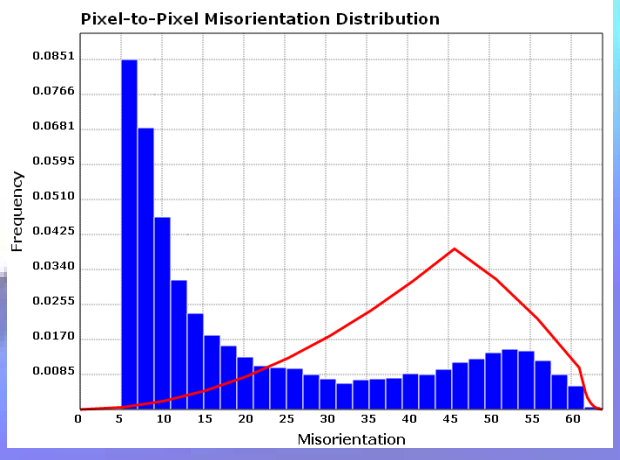
16 - Plots

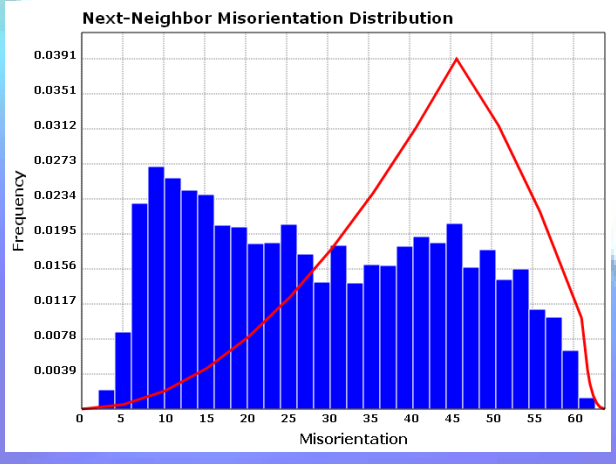
The user may plot what he wants to plot with any plotting software. Nevertheless, main informations are plotted in svg files. SVG files can be open with any internet browsers, the following plots has been checked in Google Chrome, another usefull freeware for SVG files is SVG-Edit (if you download it, simply open the html file with Firefox)

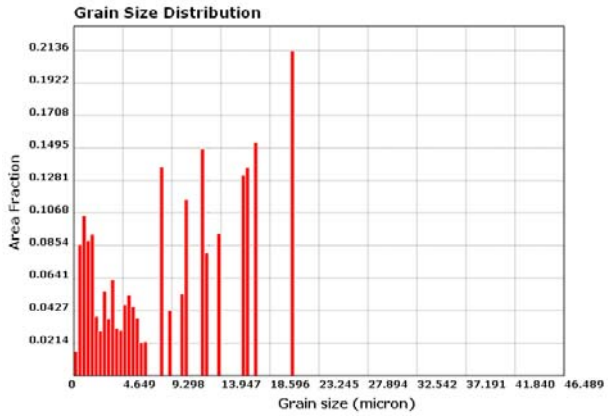
The following plots will be obtained in the case of the example ECAP_Cu_TD_1pass.ctf:

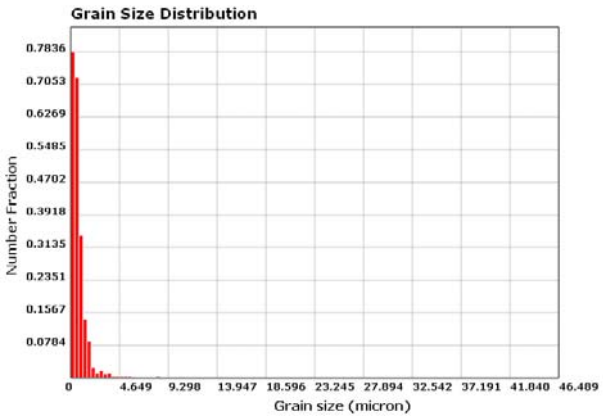










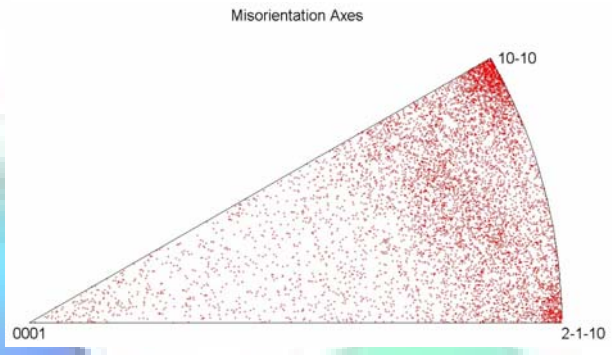


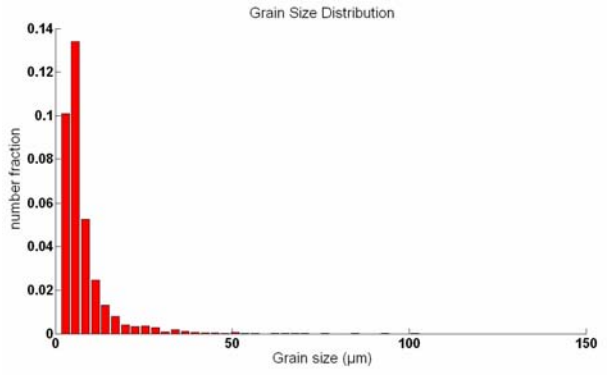
A Matlab file for plotting is also generously provided to help the user.

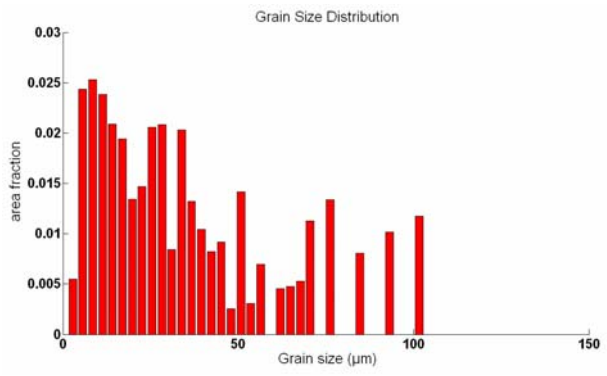
Open the file EBSDmcf.m with matlab and execute it (the correct path has to be given to Matlab).

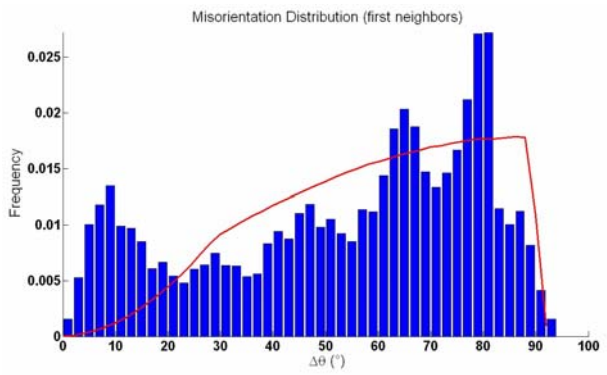
Note there is an option to smooth the MCF by kernel convolution. Set the nbkernel parameter at the beginning of the file EBSD_MCF_distrib.m (Nbkernel=0 à no kernel convolution is applied on the results, Nbkernel=1 à one kernel convolution is applied on the results, 2 à two kernel…).

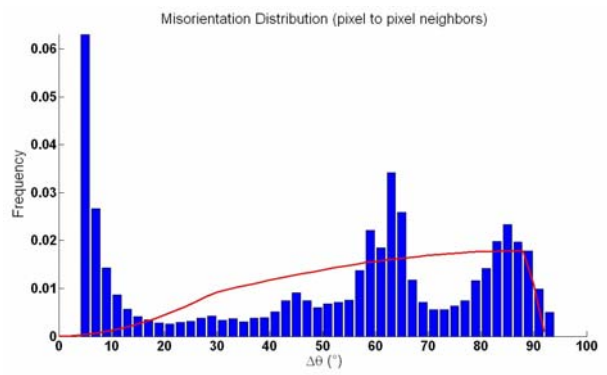
The following plots will be obtained in the case of the example Compressed_titaniun.ang.

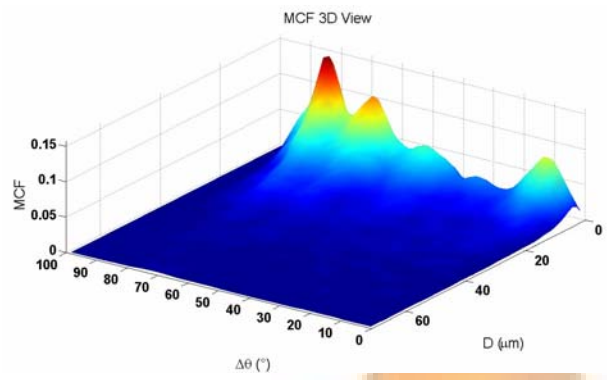


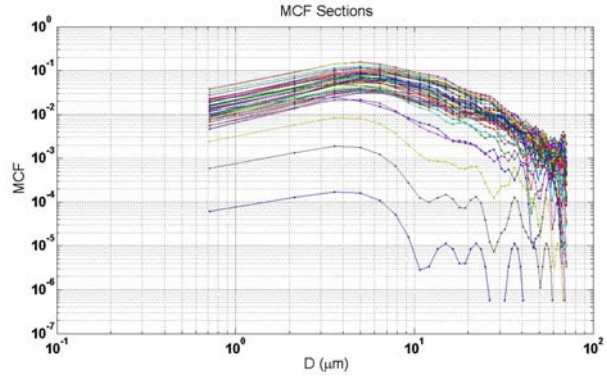

Grain Size Distribution
number fraction
Grain size (µm)


Grain Size Distribution
area fraction
Grain size (µm)


Misorientation Distribution (first neighbors)
Frequency
Δθ (°)


Misorientation Distribution (pixel to pixel neighbors)
Frequency
Δθ (°)


MCF 3D View
MCF
Δθ (°)
D (µm)


MCF Sections
MCF
D (µm)

17 - References

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